7-GeV ADVANCED PHOTON SOURCE (APS)

This completed Project is the Laboratory's largest and most-important new activity. Currently in progress is construction, of additions to this synchrotron radiation facility that is capable of producing high-intensity, tunable X-ray beams. These photon beams serve the research needs of many fields of science, including physics, chemistry, materials and surface science, biology, and medicine. The accelerator complex consists of a 200-MeV electron linear accelerator, a positron production target, a 450-MeV positron linac, an injector synchrotron to accelerate 450-MeV positrons to 7 GeV, and a 7-GeV positron storage ring of 1104 m circumference alternatively with 34 insertion-device (undulators and wigglers) beam lines and 35 or more bending magnet beam lines.

In addition, project numbers 603-608 are identified as opportunities for Excite Internships-2000 through X-ray Collaboration for Illinois Technology and Education. Applicants for internships must be currently enrolled undergraduate students at accredited two-year or four-year colleges or universities in Illinois. Applicants must be U.S. citizens or permanent resident aliens. Other selection criteria vary according to Collaborative Access Teams (CATs) involved, but include assessment of students' academic records, statements of interest, faculty recommendations, and relationship of students' interest and training to needs of particular CAT. Those considering application are encouraged to consult particular CAT web pages through the Advanced Photon Source at www.anl.gov.

600 ACCELERATOR RESEARCH AND DEVELOPMENT

Comp. Sci.
Elec. Engr.

Current research activities include accelerator physics research, charged-particle beam dynamics calculations, particle-beam transport design, measurement of accelerator magnets, fabrication and testing of vacuum system chambers, radio-frequency acceleration system measurements, accelerator diagnostic system research and development, and computer-based accelerator control system.

Mat. Sci. Mech. Engr. Phy.

601 EXPERIMENTAL FACILITIES RESEARCH AND DEVELOPMENT

Comp.
Therm.
Hydraul.
Design Engr.

These activities include research, development, and construction of instrumentation needed for the broad range of x-ray microscopy, scattering, spectroscopy, imaging, and time-resolved measurements to be performed at the Advanced Photon Source. Current activities are related to insertion devices, beam-line components, X-ray optics, detectors, novel synchrotron radiation instrumentation, and other experimental equipment useful for various research applications.

High Heat Flux Engr. Mat. Sci. Metal Engr. Phy Mech. Engr Optics

602 FACILITIES CONSTRUCTION AND PROJECT MANAGEMENT

Civil Engr.
Elec. Engr.

These activities include construction-related field engineering, safety and environmental engineering, quality assurance, and project management; civil, structural, mechanical, and electrical engineering; site improvements, and construction or modification of several buildings and utility systems.

Mech. Engr. Constr. Manag.

603 BIOPHYSCIS (BIO-CAT)

Primary foci are on the structure of partically ordered biological molecules, complexes of biomolecules, and cellular structures under conditions similar to those present in living cells. Research goals include the determination of detailed mechanisms of action of biological systems at the molecular level. Techniques used include x-ray fiber diffraction, x-ray scattering, x-ray absorption/emissions spectroscopy, and diffraction enhanced imaging. Consortium includes Illinois Institute of Technology.

604 CONSORTIUM FOR ADVANCED RADIATION SOURCES (CARS-CAT)

The consortium includes The University of Chicago, Northern Illinois University, Southern Illinois University, and Australian Nuclear Science and Technology Organization, and represents four national user groups: BioCARS for structural biology, GeoCARS for geophysical sciences, SoilEnvironCARS for soil/environmental sciences, and ChemMatCARS for chemistry and materials science. Techniques used include high pressure diffraction, microspectroscopy, microtomography, x-ray scattering, and crystallography.

605 DU PONT-NORTHWESTERN UNIVERSITY-DOW (DND-CAT)

This facility is dedicated to advancing x-ray study on new materials. Foci include the study of the atomic structures of bulk materials, the study of two-dimensional atomic structures, and polymer science and technology. Techniques include imaging, crystallography, scattering, and tomography.

606 INDUSTRIAL MACROMOLECULAR CRYSTALLOGRAPHY ASSOCIATION (IMCA-CAT)

This consortium involves crystallographic groups from 12 companies in the United States with major pharmaceutical research labs, in association with the Center for Synchrotron Radiation Research at the Illinois Institute of Technology. A large fraction of the research is proprietary. Techniques include multiwavelength anomalous diffraction.

607 MATERIALS RESEARCH (MR-CAT)

Illinois Institute of Technology is among four universities and one major corporation (BP-Amoco) involved with this collaboration. Foci includes studies of advanced materials in situ as a means of characterizing their structure and electronic properties, as well as understanding their preparation. Primary techniques include wide- and small-angle scattering, single-crystal and powder diffraction, absorption spectroscopy, reflectivity, standing waves, diffraction anomalous fine structure, and time-dependent and microfocus techniques.

608 UNIVERSITY-NATIONAL LABORATORY-INDUSTRY (UNI-CAT)

In these sectors, The University of Illinois at Urbana-Champaign is teamed with Oak Ridge National Laboratory, the National Institute of Standards and Technology, and UOP Research and Development. This is a multi-purpose scattering facility capable of high-resolution scattering with excellent energy resolution and beam-focusing optics serving studies in materials, physics, chemistry, biology, and geology.

ARGONNE NATIONAL LABORATORY-WEST (ANL-W)

Argonne National Laboratory-West (ANL-W) is located in Southeastern Idaho on the Idaho National Engineering and Environmental Laboratory site. ANL-W is part of Argonne National Laboratory (ANL) located near Chicago. The ANL-W site is about 35 miles west of Idaho Falls, Idaho. ANL is a non-profit research Laboratory operated by The University of Chicago for the United States Department of Energy. A broad range of national problems are solved through ANL research and development activities.

Research at ANL-W is focused on areas of national concern including those relating to energy, nuclear safety, spent nuclear fuel, nonproliferation, decommissioning and decontamination technologies, and similar work. Typically, basic research is conducted at the main Laboratory near Chicago, with large-scale testing and development at the Idaho site. Nuclear fuel development, post irradiation examinations, characterization, and development of dry storage for spent fuels and other materials are but some of the accomplishments at ANL-W.

609 EXPERIMENTAL BREEDER REACTOR - II

Comp. Sci.

Elec. Engr.

Indus. Safety

Mat. Sci.

Math.

EBR-II served as the nation's R&D center for fast reactor technology from August of 1964 to September of 1994. EBR-II demonstrated the feasibility of a fast reactor for central power station use, served as an irradiations facility for the development of fuels and materials for nuclear plants, and performed special fuels safety tests such as Run Beyond Cladding Breach experiments in an international program.

EBR-II led the world in demonstrating that reactor safety can be an inherent part of the system design through using natural phenomena that operators cannot defeat, such as thermal expansion and convective flow. Inherent safety characteristics were demonstrated in specials tests of EBR-II in 1986, which led to including passive safety features in new nuclear reactor designs.

EBR-II is now defueled. The EBR-II shutdown activity also includes the treatment of its discharged spent fuel using an electrometallurgical fuel treatment process in the Fuel Conditioning Facility, located next to the EBR-II.

The cleanup process for EBR-II includes the removal and processing of the sodium coolant, cleaning of the EBR-II sodium systems, removal and passivating of other chemical hazards and placing the deactivated components and structure in a safe condition.

610 FUEL MANUFACTURING AND FUEL ASSEMBLY FACILITIES

Chem. Engr.

Comp. Sci.

Envr. Sci.

Mat. Sci.

Fuel Manufacturing Facility (FMF) and the Fuel Assembly Buildings (FASB) had, as a mission the fabrication of unirradiated fuel for the Experimental Breeder Reactor II. They are currently used for the development and testing of high density low enriched fuels for research reactors. This is part of the safeguards and arms control program. They are also used to develop and verify the suitability of waste forms resulting from the treatment of EBR-II spent fuel, for eventual placement in a repository. The FMF is a secure facility with state of the art safeguards for fissile material. It was recently featured in a joint demonstration of remote monitoring of the safeguards between the United States and the Kurchatov Institute in Russia.

611 FUEL CONDITIONING FACILITY

Chem. Engr. *Comp. Sci.* *Elec. Engr.* *Indus.*

The Fuel Conditioning Facility (FCF) plays the central role in EBR-II spent fuel treatment. After major renovation, the FCF is being used to treat EBR-II spent fuel as a technology demonstration. Successful treatment of EBR-II spent fuel may mean that the process could be used for treatment of other problematic DOE spent fuel types, resulting in common final waste forms for disposal.

The FCF consists of special cells designed to handle highly radioactive materials such as spent fuel. One cell has an air atmosphere, the other has an (non-reactive) atmosphere of argon gas. Process equipment, located in the cells, is operated remotely which allows the fuel treatment process to be safely controlled and monitored.

Safety Mat. Sci. Math. Mech. Engr. Nucl. Engr. Phy.

612 ANALYTIC LABORATORIES

Chem. Chem. Engr. *Comp. Sci.* *Mat. Sci.*

The AL is a state of the art laboratory complex which includes shielded analytical hot cells, general purpose laboratories, a glovebox laboratory, mass spectrometry laboratories, and alpha, beta, and gamma-ray counting rooms. Laboratory equipment includes state-of-the art mass spectrometers, inductively coupled plasma-atomic emission spectrometers, atomic absorption spectrometers, counting equipment, ion chromatographs, and gas chromatographs. Capabilities include the analysis of total and isotopic U, Pu, Am, Np, the measurement of radioactive fission and activation products, major and minor components in solutions of highly radioactive samples, and the characterization of radioactive, hazardous, and TRU waste.

Nucl. Engr.

613 HOT FUEL EXAMINATION FACILITY

Chem. Chem. Engr. *Comp. Sci.* *Elec. Engr.* *Indus. Safety* *Mat. Sci.*

The Hot Fuel Examination Facility (HFEF), is a versatile modern hot cell facility that is operated to characterize and package spent fuel and radioactive waste materials, and to provide some waste-form treatment operations. One such operation is where fission products and transuranic elements will be bound in a highly stable mineral structure (sodalite) for disposal in a repository. The cells are adaptable to multi-use configuration, depending on specific needs. The cells in HFEF include an air-filled cell, used for decontamination of cell equipment, and the main argon filled cell. The argon cell is used for destructive and non-destructive examinations of irradiated fuels and materials. HFEF houses what is likely the largest and most versatile hot cell of its kind in the world. Fuels of virtually all kinds have been examined in the HFEF, both by non-destructive and destructive methods, including neutron radiography, gamma scanning, physical measurements, scanning electron and optical microscopy exams, etc. HFEF also includes the Waste Characterization Area where characterization and repackaging of mixed hazardous waste to be transported to the Waste Isolation Pilot Plant facility in New Mexico is done.

Math. Mech. Engr. Nucl Engr.

614 TRANSIENT REACTOR TEST FACILITY

Comp. Sci.
Math.
Mech. Engr.
Nucl. Engr.
Phy.

Transient Reactor Test Facility (TREAT) is a uranium-oxide fueled, graphite-moderated and air-cooled reactor designed to produce short controlled bursts of nuclear energy for safety testing of nuclear fuels and materials. Accident conditions can be simulated up to and including melting or even vaporization in test specimens, while leaving the reactor and the "driver" fuel undamaged. TREAT is presently in standby, with a number of potential missions for the facility.

The TREAT driver fuel, consisting of finely divided uranium oxide in a carbon and graphite matrix, has a high heat capacity which enables it to withstand the transient tests. The reactor's air-cooling system is adequate for cooling the core to ambient temperature in a matter of hours after a transient test, or for steady-state operation at up to 120 kilowatts. The nominal peak power allowed in transient tests is 18,000 megawatts of thermal power greater than five times the largest nuclear power plants.

TREAT has served as a unique test facility for both national and international needs.

Recently, the large highbay and open floor space in the TREAT facility was used for testing of a Plasma Hearth Process (PHP), a thermal treatment process for radioactive wastes. The plasma hearth process melts drums of radioactive waste into relatively small chunks of glass and metal.

615 ZERO-POWER PHYSICS REACTOR

Comp. Sci.
Math.
Mech. Engr.
Nucl. Engr.
Phy.

The Zero-Power Physics Reactor (ZPPR) is a test facility for the mock up and physics testing of full sized reactor core designs. Testing was done by assembling fissile materials in a configuration closely resembling a particular design under consideration except that the reactor assembly was operated at very low power levels. ZPPR operation was normally limited to a few to a hundred watts. ZPPR critical assemblies were put together from rectangular "building blocks" of fuel (including plutonium or uranium), coolant, and various structural materials. Information gained from ZPPR was used as input to computer codes for reactor design. The ZPPR is now shut down, however, the fuel storage vault is used to safely store ZPPR fuel. In addition, a Gas Generation test is being conducted in the ZPPR facility to determine what if any, gases will be generated in conditions simulating long-term residence of waste buried in the WIPP facility.

616 NEUTRON RADIOGRAPHY REACTOR

Comp. Sci.
Mat. Sci.
Nucl. Engr.

The Neutron Radiography Reactor (NRA1) is a 250-kW TRIGA nuclear reactor that provides neutron radiography capability. One port allows specimens to be lowered from the main HFEF argon cell to intersect a collimated neutron beam from the reactor. A second neutron radiography station, outside of the argon main cell, enables radiography to be conducted without introducing specimens into the HFEF argon cell. In addition, there is one in-core irradiation position for performing irradiation experiments and for activating gamma sources.

A neutron generator in one of the shielded cells is used to perform non-destructive analysis and assay experiments. These include assay of waste forms and fuel elements.

617 RADIOACTIVE SCRAP AND WASTE FACILITY

Envr. Engr.
Waste Mgmt. Engr.
Chem. Engr.

The Radioactive Scrap and Waste Facility (RSWF) provides the fully permitted interim storage capability for a wide variety of experimental spent fuels and radioactive scrap. RSWF is a simple underground facility with individually enclosed and shielded storage locations for spent fuel and radioactive materials. Radioactive contents of each storage located are isolated by a stainless steel safety grade barrier enclosing a carbon steel canister containing the radioactive material. A protective outer silo contains the canister payload. RSWF provides the temporary storage of radioactive and mixed hazardous material generated at ANL-W or which may be sent to ANL-W for research purposes.

Corrosion Engr.

618 MICROSCOPY LABORATORY

Chem. Engr.
Math Sci.
Nucl. Engr.
Phy.

The ANL-West Electron Microscopy Laboratory was established in 1998 to provide a facility for the detailed characterization of radioactive and non-radioactive materials. Instruments in the facility include scanning and transmission electron microscopes which are used for imaging and identifying microstructural features such as phases and irradiation-induced defects. Such characterization is important to understand how radiation environments or material processing techniques affect material properties and performance. Techniques commonly employed include electron diffraction and microchemical analysis using energy-dispersive and wavelength-dispersive spectrometers. The facility is also equipped with flume hoods and glovebox to house specialized equipment for preparing samples of radioactive materials for subsequent characterization.

619 NUCLEAR MATERIAL SAFEGUARDS AND NONPROLIFERATION

Comp. Sci.
Elec. Engr.
Nucl. Engr.

Argonne National Laboratory-West is involved in a number of nuclear material safeguards and nonproliferation activities. Included in these areas are projects involving advanced software development, e.g., expert systems, statistical signal processing, artificial intelligence applications, for safeguard data analysis and material characterization. The Laboratory operates the Safeguard Technology Evaluation Laboratory where evaluation of plutonium monitoring and surveillance systems are evaluated under static and transient conditions. Opportunities exists in the areas of software development, electronic system design and analysis and nondestructive assay and testing of packaged nuclear materials.

Phy.

620 NONDESTRUCTIVE ASSAY AND NONDESTRUCTIVE EVALUATION

Elec. Engr. Nucl. Engr. Phy.

Argonne National Laboratory is involved in several nondestructive assay (NDA) and nondestructive evaluation (NDE) projects. NDA and NDE are integral parts of the most nuclear material related activities including arms control and nuclear nonproliferation, spent fuel management, waste management and nuclear facility operations. ANL has programs ongoing involving both active and passive interrogation of irradiated materials involving gamma ray spectroscopy, neutron coincidence and delayed neutron counting, neutron radiography and neutron transmission analyses. Resources include a full compliment of gamma ray and neutron measurement devices and associated electronics, nuclear measurements laboratories and associated materials, a 14 MeV neutron generator and a 250 Kw TRIGA reactor with associated neutron radiography laboratories. Advanced data processing applications for NDA data analyses are also of importance.

621 ANL-WEST ENGINEERING SUPPORT GROUPS - A AND B

Chem.

The support functions at ANL-West include many site-wide services to the major facilities.

Civil Engr. Comp. Sci.

a. Engineering provides engineering design and project management support for new buildings, building additions and modifications to the physical plant facilities. The functional specialties include project management, mechanical, electrical, civil, architectural and structural engineering.

Elec. Engr. Indus. Safety Mat. Sci. Mech. Engr. Radio-chem.

b. The Environment, Safety and Waste Management (ESM) Department is responsible for the environment, safety and health, and waste management for the ANL-W Site. The mission is to ensure the implementation of all Laws (Federal and State), Regulations, DOE Orders and good practices required to ensure the quality of the environment, safety and health of the employees and general public.

The safety responsibilities include radiation protection, fire protection, industrial hygiene, and industrial safety. Environment and waste management includes the control of hazardous radioactive and radioactive mixed waste; control of emissions; and ESM manages the DOE Environmental Restoration and Waste Management. (ER/WE)_ Five Year Plan which designates funding and established the context within which environmental cleanup, waste operations and research and development activities at DOE sites are performed.

BIOSCIENCES DIVISION (BIO)

Research in this Division is aimed at defining the biological and medical hazards to humans from energy technologies and new energy options. Health-related studies are supported by fundamental research in scientific disciplines, including molecular and cellular biology, crystallography, biophysics, genetics, radiobiology, biochemistry, chemistry, and environmental toxicology. The research involves the integration of findings from investigations at the molecular, cellular, tissue, organ, and whole-animal levels, with the ultimate aim of applying these findings to problems of human health. The Division is organized into two scientific sections (Biophysics, and Functional Genomics), plus a Structural Biology Center that operates two beamlines at the Advanced Photon Source. Each section comprises several research groups with considerable interaction occurring among all groups. Divisional support facilities include an editorial office, a computer center, a biomedical library, and an instrument design and maintenance shop.

BIOPHYSICS SECTION

622 MACROMOLECULAR INTERACTIONS

Bio.
Biochem.
Molec. Bio.
Biophy.

A major research goal in biological science is to understand the relationship between the amino acid sequence of a protein and its three-dimensional structure, stability, and function. Because the interactions between the amino acids within a protein obey the same laws of physics that control interactions between proteins, study of the self-association properties of immunoglobulin light chains is relevant to the fundamental properties of all proteins. Antibody light chains are produced in large quantities by patients who have myeloma, a neoplasm. Because the proteins produced by two patients will be similar in three-dimensional structure but will differ in amino-acid sequence, differences in self-association (under various conditions of pH, ionic strength, and temperature) can be related to the physics that determines the protein structure and function. In addition, these studies provide increased understanding of the biophysical properties of these proteins that lead to disease complications in many patients. We are using site-specific mutagenesis of light chains and molecular dynamics simulations to help analyze experimental results.

623 PROTEIN CRYSTALLOGRAPHY AND MOLECULAR MODELING

Chem.
Biochem.
Biophy.
Comp. Sci.

The principal aims of this program are the isolation and characterization of biologically important macromolecules, the determination of their detailed three-dimensional structures in crystalline and aqueous phases, and the correlation of structure with biological function. The biomolecules under study include various antibodies and the bacterial photosynthetic reaction center. The techniques used in this program are taken from a variety of disciplines including molecular biology, protein chemistry, chromatography, immunochemistry, protein crystallography, computer modeling of protein structures, and computer simulation of macromolecular interactions. Major equipment includes a rotating anode X-ray generator with an R-axis#2 data collection system, interactive computer color graphics terminals for manipulating macromolecules in three dimensions, and computer-interfaced high-performance liquid-chromatography and capillary electrophoresis systems.

624 SBC/APS USER FACILITY

Biochem. *Biophy.* *Comp. Sci.* *Synch. Radia.*

This program applies modern crystallographic methods to rapidly determine structures of biological macromolecules-proteins and nucleic acids-as single molecules, as multicomponent complexes, and complexed with smaller molecules. A significant effort in this program is directed toward improving the methods for crystallographic investigation of macromolecular structure, by developing new and better methods and instruments to measure, process, and analyze diffraction data using cryocrystallography. The program operates two advanced x-ray beamlines at the Advanced Photon Source, for tuned, monochromatic x-ray diffraction data collection that is used to determine crystal structures. Crystal structures are being studies of chaperone proteins which direct the folding of nascentproteins, important enzymes from pathogenic and thermolphilic organisms, and nucleic acids. Structures of proteins derived from genomic analysis as part of our structural genomic initiative are being determined at this facility. Major equipment includes rotating-anode x-ray generator, with imaging plate detector, two CCD-based area detectors, modern workstations with large capacity data-storage disks, several interactive graphics workstations for molecular modeling, HPLC, FPLC, and ectrophoresis equipment, and all necessary facilities and equipment for molecular biology, molecular genetic manipulations of DNA, protein purification and crystallization.

625 PROTEIN ENGINEERING

Bio. *Biochem.* *Biophy.* *Genetics* *Molec. Bio.*

This program is aimed at understanding how a protein's three-dimensional structure defines its function. Our work is focused on the bacterial photosynthetic reaction center, a transmembrane protein complex that functions in the process by which light energy is converted into chemical energy. In order to understand how the structure of this protein defines its functions, specific changes are being made in its primary amino acid sequence by site-directed mutagenesis. Several techniques of molecular biology and genetics are used to create mutations, and the mutant proteins are then expressed in the *Rhodobacter* species of photosynthetic bacteria. Changes in the functional properties of purified mutant proteins are then characterized by various types of spectroscopy. Mutant proteins of special interest are selected for crystallization and structure determination by x-ray crystallography. Other projects involve the development of systems for the heterologous expression, purification, and crystallization of additional proteins for structure determination. Techniques involved include gene cloning with plasmid vectors, gel electrophoresis, PCR amplication of DNA sequences, DNA sequencing, protein expression and purification, spectroscopy, and bioassay of mutant phenotypes.

626 STRUCTURAL STUDIES OF MACROMOLECULAR ASSEMBLIES

Biophy.
Molec. Bio.
Biochem.

Recognition of biological macromolecules and their interaction and assembly into larger supermacromolecular structures are at the heart of many important processes in molecular and cellular biology. For example, macromolecular assembly occurs in protein biosynthesis, in the recognition of receptors by protein hormones, in the folding of proteins, and in the recognition of and binding to nucleic acids by proteins that regulate the expression of genetic information. We are studying macromolecular assemblies at the atomic and molecular levels by x-ray crystallography, in particular the protein-protein interactions of molecular chaperones of the hsp60 and hsp70 classes and large oligomeric enzymes.. Because the crystals of macromolecular assemblies are usually small and fragile and have large unit cell dimensions, they diffract weakly. Furthermore, these crystals have large, complex structures and their structure determination is experimentally demanding. These studies take advantage of the Advanced Photon Source at Argonne. The techniques being used include molecular biology and biochemistry protein crystallography, x-ray diffraction, high-performance liquid chromatography, and electrophoresis.

FUNCTIONAL GENOMICS SECTION

627 PROTEOMICS

Bio.
Biochem.
Comp. Sci.

Two-dimensional gel electrophoresis coupled with computerized image and data analysis is being used to characterize the normal protein composition of cells and to detect changes in response to environmental pressures. Current studies are focused on the analysis and identification of proteins produced by hyperthermophilic organisms. In addition to two-dimensional gel electrophoresis of proteins (isoelectric focusing by sodium dodecyl sulfate polyacrylamide gel electrophoresis), this project involves the use of image and data analysis algorithms, World Wide Web databases, and mass spectrometry. The construction and maintenance of interactive Internet databases is an important part of the data presentation for this project.

628 GENOME TECHNOLOGY

Biochem.
Molec. Bio.

We are developing DNA sequencing technology using modular primers that eliminates the need for primer synthesis, the main bottleneck in primer walking. Modular primers are assembled from three 5-mer, 6-mer, or 7-mer modules selected from a presynthesized library of as few as 1,000 oligonucleotides. The three modules anneal contiguously at the selected template site and prime there uniquely, even though each is not unique for the most part when used alone. This technique is expected to speed primer walking 20- to 50-fold and to reduce sequencing costs by a factor of 5-15. The instant availability of the primers enables closed-loop automation of the complete cycle of walking sequencing, and a closed-loop process largely eliminates the human intervention as a source of errors and complications.

629 BIOCHEMICAL TOXICOLOGY

Bio.
Biochem.
Chem.
Tox.

This research program is designed to investigate health effects of toxic metals to which humans may be environmentally or occupationally exposed. One research area focuses on the role of pregnancy, lactation, or ovariectomy in the susceptibility of animals to bone loss after cadmium exposure. Mechanisms of cadmium action on bone are studied in isolated bone cells in culture and in the RNA isolated from bones. Molecular pathways of cadmium action are investigated with reverse transcriptase-polymerase chain reaction for specific genes known to influence bone resorption and by differential display to identify unknown genes. Measurements of bone-related cytokines and resorption markers in blood and urine are measured by enzyme-linked immunosorbent assays and by high-performance liquid chromatography. Another research area focuses on the biochemical pathways for metabolizing toxic heavy metals, including their uptake and tissue deposition. The role of metallothionein, a metal-binding protein, is studied using normal and metallothionein-deficient mice. Measurements of calcium and cadmium content in tissues are performed using atomic absorption spectroscopy.

630 MOLECULAR RADIOBIOLOGY

Bio.
Biochem.
Molec. Bio.

Molecular studies focus on the effects of exposure to environmental stresses (such as radiation) on the activation of specific gene sequences in cells. This work will examine genes activated and repressed by ionizing radiation and will identify protective and repair mechanisms used by cells following exposure to radiation. Some experiments are examining the genetic basis for radiation sensitivity in a mutant mouse strain. In addition, mechanisms of radiation-mediated carcinogenesis are being explored at the molecular level using preserved tissues. Techniques used include Northern and Southern blotting procedures, nucleic-acid hybridization, cDNA cloning, polymerase chain reaction amplification, gel-shift assays and transcription run-on assays.

BIOTECHNOLOGY (BIOT)

Biotechnology research at Argonne National Laboratory deals with applying biology and biochemistry principles and breakthroughs to problems of national interest. In health-related studies, researchers advance the development and use of biological microchips, or biochips, to speed DNA sequencing of human genes and to identify organisms and toxins of bacteria, viruses, and other microorganisms. In collaborative efforts, Laboratory staff study the effects of biochemicals to control leukemia and other cellular malignancies, target enzymes to screen for new drugs, and study cellular replication, differentiation, apoptosis in tumors. Engineers promote industry processes to produce environmentally friendly "green" solvents, support an emerging agriculture-based chemical industry, and develop biocatalytic systems for the production of chemicals from renewable resources through numerous industry/government partnerships. And to help clean the environment, researchers continue to develop and test novel technologies to remove, detoxify, and recover heavy metals and other unwanted entities from pipelines, soils, groundwater, and aqeuous waste streams.

HEALTH

631 BIOCHIP TECHNOLOGY

Bio-Chem.
Chem.
Comp. Sci.
Gene.
Mole. Bio.

A commercial joint-research project among Motorola Incorporated, Packard BioScience Company, and Argonne National Laboratory works toward commercializing and marking advanced biological microchips, or biochips, and related analytical technologies to permit faster and more efficient detection of mutations in genetic information encoded in DNA, the macromolecule of human genes which is packaged in the chromosomes in cells. Polyacrylamide micro-gel pads – thousands of them on a single one-square-inch glass slide – act as microscopic laboratory test tubes in which biological targets can be tested against chemical compounds. With known strands fixed in place, robots and other automated equipment allow researchers to use the slides as templates to test and decode unknown DNA samples. Primary applications include medical diagnostics, drug discovery and medical treatment, environmental restoration, and agricultural-product testing.

632 BIOCHIP TECHNOLOGY – ADVANCED APPLICATIONS

Bio-Chem.
Chem.
Comp. Sci.
Gene.
Mole. Bio.

Argonne and Russian scientists are exploring and expanding the biochip's wide range of applications in:

a. DNA sequence analysis and proofreading.
b. Analysis of changes in genetic makeup (mutations),
c. Analysis of population differences in genetic coding (polymorphism),
d. Identification of bacteria, viruses, and other microorganisms,
e. Analysis of gene expression in health, disease, and drug treatment,
f. Advanced medical diagnostic and monitoring of treatment, and
g. Detection of genetically engineered biothreat agents.

633 CELL GROWTH AND DIFFERENTIATION

Bio-Chem.

This research seeks to examine the molecular events that govern cellular replication, differentiation, and programmed cell death (apoptosis) in normal and tumor cells.

Cell Bio.

a. Chemicals are being studied for their roles in signal transduction events (such as activation of protein kinases, production and interaction of adhesion molecules, or inhibition of protein phosphatases) that alter cellular replication, differentiation, or apoptosis.

Gene.

b. Laboratory staff are characterizing human genes that code for proteins that modulate cellular replication, differentiation, and or apoptosis in normal and tumor cells.

Mole. Bio.

c. Research on inosine 5'-monophosphate dehydrogenase (IMPDH), a target for immunosuppressive and anticancer drugs, focuses on its regulation and structure.

Results could provide the foundation for developing highly specific chemicals that could be used as pharmaceutical agents.

[Also, see related listing under the Biosciences Division.]

INDUSTRY

634 ENVIRONMENTALLY FRIENDLY SOLVENTS

Biochem. Engr. Chem. Engr. Chem. Envr. Engr. Micro-Bio.

Widely used chemical solvents, such as chlorofluorocarbons, damage the earth's ozone layer, while chloroform and trichloroethylene remain the most common groundwater pollutants. Ethyl lactate, a non-toxic and biodegradable solvent, occurs naturally in beer, wine, and soy products and is approved as an additive by the U.S. Food and Drug Administration. Argonne has developed a technology that can sufficiently reduce the cost of the environmentally benign solvent, ethyl lactate, to make it competitive in the marketplace against toxic solvents. A novel membrane-based process to produce lactate esters is being developed through an industry/government initiative.

[Also, see related listing under the Energy Systems Division, Center for Industrial Technology Systems.]

635 BIOCATALYTIC SYSTEMS FOR THE PRODUCTION OF CHEMICALS FROM RENEWABLE RESOURCES

Bio-Chem. Biochem. Engr. Chem. Engr.

Through industry/government partnerships, Argonne is part of a consortium to develop a new, integrated process approach for synthesizing industrial chemical intermediates and derivatives from renewable biomass. Argonne's role is to apply its technical expertise in genetic engineering, bioprocess engineering, and polymer development to targeted products and processes. For example, Argonne is improving fermentation efficiency by using conventional and genetic techniques to develop superior succinic-acid-producing organisms. Its purification process uses advanced desalting and water-splitting electrodialysis technologies.

Chem.

[Also, see related listing under the Energy Systems Division, Center for Industrial Technology Systems.]

Mole. Bio.

636 PHYTOREMEDIATION

Agro-sci.
Bio-Chem.
Civil Engr.
Ecol.
Engr.
Geol.
Micro-bio.

Phytoremediation, the engineered use of green plants to remove, contain, or render harmless such environmental contaminants as heavy metals, trace elements, organic compounds, and radioactive compounds, is an emerging cleanup technology for contaminated soils, groundwater, and wastewater that is both low-tech and low-cost. In 1995, greenhouse experiments on zinc uptake in hybrid poplar were conducted to confirm and extend field data from Applied Natural Sciences, Inc. in a collaborative research and development effort. Analyses indicate that part-per-million levels of zinc are totally sequestered by the plants through the root system in several hours in a single pass. Similar experiments with a grass show similar patterns partitioning and sequestration as the poplar experiments but with the growth and transpiration more suppressed. Current studies include groundwater remediation and field demonstrations for the uptake of halogenated organics in hybrid poplar.

[Also see related listing under the Energy Systems Division, Center for Environmental Restoration Systems]

637 FOAMS ACCELERATE REMEDIATION OF SOIL AND GROUNDWATER

Chem.
Chem. Engr.
Envr. Engr.

Argonne is experimenting with specially designed foams to increase the applicability of *in-situ* bioremediation to clean up soil and groundwater contaminated by nonaqueous-phase organic liquids (NAPLs), such as tricholoehylene and carbon tetrachloride, or polyaromatic hydrocarbons, such as chrysene, benz(a)anthracene, anthracene, fluoranthene, and phenanthrene. Although foams have been applied in deep subsurface formation for improved flow control during enhanced oil recovery, they have not yet been systematically applied to environmental remediation problems closer to the surface. Argonne researchers are exploring the opportunity to adapt and mature this existing foam technology by integrating it with bioremediation, also called “bioaugmentation,” (either *in-situ* or *ex-situ*) for the cleanup of hazardous waste.

[Also see related listing under the Energy Systems Division, Center for Environmental Restoration Systems]

638 PHOTOCATALYSTS TO TREAT AQUEOUS WASTE STREAMS

Chem.
Chem. Engr.
Civil Engr.
Engr.

Argonne is developing and testing unique photocatalysts to remove, detoxify, and recover heavy metals (such as lead, cadmium, chromium, copper, mercury, and arsenic) from aqueous waste streams, while simultaneously destroying organic compounds (such as carbon tetrachloride and trichloroethylene). If successful, this technology would represent a significant breakthrough for the treatment of heavy-metal-contaminated waters at U.S. DOE and industrial sites. Because the metals are recovered in metallic form, heavy-metal toxicity is minimized and the number of steps required for recovery is reduced. In this approach, Argonne chemists are using organic modifiers at the surface of nanosized particles of titanium dioxide (TiO_2) colloids that are selectively optimized for photochemical reactivity towards toxic metal ions. In parallel research, Argonne engineers are conducting batch, bench-scale experiments on aqueous solutions containing various metal and organic contaminants to determine process kinetics and optimal treatment conditions.

[Also see related listing under the Energy Systems Division, Center for Environmental Restoration Systems]

CHEMICAL TECHNOLOGY DIVISION (CMT)

This Division is a multidisciplinary research and development organization in which engineers and scientists bring their diversified talents to bear on a wide variety of problems, most of which are related to the nation's energy and environmental needs. Currently, emphasis is being given to the development of near-term and advanced batteries; fuel-cell research and development; development of separation processes for radioactive, mixed, and hazardous wastes; studies of reactor-fuel processing, geochemical studies, and radioactive-waste management; and environmental chemistry studies. All Chemical Technology Division projects are backed up by strong basic research. Thermodynamic studies and studies of phase relationships, molecular structure, surface chemistry, analytical chemistry, metallography, mathematical modeling, and reaction kinetics are carried out to gain a better insight and understanding of the underlying phenomena upon which major engineering projects are based.

FUEL CELL R & D

639 MOLTEN CARBONATE FUEL CELL DEVELOPMENT

Ceram.
Chem.
Chem. Engr.
Metal. Engr.
Phy.

The objective of the program is to provide solutions to current technical problems identified in the DOE Molten Carbonate Fuel Cell (MCFC) Program. Research is concentrated on materials and component development for, and testing and modeling of, MCFC. Research is related to development of corrosion-resistant materials (base materials or coatings and composites) and new electrode and electrolyte materials and structures. It may involve characterization of materials and components such as vapor pressure of electrolytes; determination of electronic and/or ionic conductivity of various components; crystal defect studies (e.g., conductivity, thermogravimetric analysis, valence state analysis); and analysis of in-cell behavior of components (e.g., sintering, migration, phase stability, morphological changes, and chemical stability). Modeling research is being done and involves experimental verification as well as model development and application.

640 POLYMER ELECTROLYTE FUEL CELL DEVELOPMENT

Chem.
Chem. Engr.
Mat. Sci.
Phy.

Because of its low temperature and solid electrolytes, the polymer electrolyte fuel cell (PEFC) is being developed for mobile power applications, such as passenger vehicles. PEFCs are fueled by hydrogen, which is produced through the reforming of alcohols and other fuels. The reforming process results in contamination of the hydrogen by carbon monoxide, causing degradation of the PEFC performance. The goal of this program is to develop an electrode catalyst for the fuel cell which will run on carbon monoxide-contaminated hydrogen. This project involves the use of basic electrochemical techniques to determine the hydrogen oxidation kinetics and CO tolerance of newly developed electrode materials. It also involves the construction and electrochemical testing of fuel cell assemblies and post-test examination of the cell materials by scanning electron microscopy (SEM) and other techniques. Major equipment includes: electrochemical instrumentation (potentiostat and galvanostat), AC impedance system, scanning electron microscope, and personal computers.

641 FUEL PROCESSING FOR FUEL CELLS

Chem. *Chem. Engr.* *Mat. Sci.*

Low-temperature polymer electrolyte fuel cells are being developed for use in light-duty vehicles and stationary applications. These fuel cells operate best with hydrogen. However, the lack of a hydrogen supply infrastructure and the low energy density of hydrogen storage technology have created a need for compact and lightweight fuel processors that can convert available liquid fuels or natural gas into hydrogen-rich gas. These fuel processors involve a number of unit operations and processes and require new and more advanced technologies (catalysts, reactor designs, integration methods, etc.) for the various applications. This project undertakes the development of all aspects of the fuel processor and includes the catalytic reforming process, sulfur and carbon monoxide (a byproduct of the reforming reaction) removal and cleanup, and the integration of all the components into a compact hardware. All of these activities are pursued through mathematical modeling and experiment. Major experimental equipment includes a gas chromatograph, mass spectrometer, IR analyzer, thermal conductivity analyzer for hydrogen, CO chemisorption analyzer, apparatus for BET surface area measurement, and catalytic reactor test stands. Material characterizations are performed with scanning electron microscopy, X-ray diffraction, and chemical assay. Reactor and systems modeling are done with the Gctool computer code in the Technology Development Division, as well as with various software used for thermodynamic and kinetic calculations.

642 SOLID OXIDE FUEL CELL DEVELOPMENT

Ceram. *Chem.* *Chem. Engr.* *Metal Engr.* *Phy.*

Research activities are concentrated on the development of a new type of solid oxide fuel cell (SOFC). Efforts are directed toward defining materials and fabrication methodology that will achieve the desired structure and properties for the electrolyte and electrodes. The project involves the characterization of high-temperature, inorganic materials by means of X-ray, surface area, electron microscopy, and other techniques. The project also involves the fabrication and characterization of ceramic structures using tape casting, slip casting, extrusion, complex impedance measurements, and other techniques. There is a continuing effort to enhance understanding of the fundamental mechanisms of fuel-cell operation and to improve fuel-cell design and operation. Major equipment includes: tape caster, furnaces, AC impedance system, computer, and scanning electron microscope.

643 NOVEL MATERIALS FOR USE IN SOLID-STATE FUEL CELLS

Ceram. *Ceram. Engr.* *Chem.*

This research effort is directed toward the development of new materials for use in a moderate-temperature-range (500-800°C) fuel cell. Studies are currently being conducted to find new, highly conductive materials for use as the anodes, cathodes, electrolytes, and interconnects. Effort involves synthesis of materials, sintering and processing of materials, and characterization of electrochemical and chemical properties. Major equipment includes: frequency response analyzer, differential thermal analyzer, dilatometer, optical microscope, scanning electron microscope, electrochemical analytical equipment, and computer-controlled data acquisition and reduction.

644 GLASS HYDRATION STUDIES

Archeo.
Chem.
Mat. Sci.

When glass is contacted by water vapor or liquid water, alteration reactions occur. Water penetrates into the glass, forming a hydration layer, and displaced atoms diffuse to the glass surface and form minerals. These reactions are of interest to archaeology since hydration aging dating of natural glasses is a subject not well understood. These reactions are also important to nuclear waste management since such surface alteration will affect the waste form behavior over extended storage periods. This program investigates the kinetics and mechanisms of these reactions using surface analytical techniques such as scanning electron microscopy. Major equipment includes: scanning electron microscope, transmission electron microscope, energy dispersive X-ray analyzer, laser Raman spectrometer, and Fourier-transform infrared spectrometer.

645 NUCLEAR WASTE TESTING

Chem.
Chem. Engr.
Envr. Sci.
Nucl. Engr.

The aim of this program is to determine the magnitude and composition of the source term for nuclear wastes in an environment similar to that expected for the candidate repository site at Yucca Mountain. Projects include tests on spent UO_2 fuels and waste glass, which are conducted in hot cells, and the analysis of the solid phases, colloids, and solutions obtained through intermittent sampling of the tests. A participant assisting this group would have opportunity to learn state-of-the-art techniques for studying the long-term corrosion of radioactive waste materials.

646 SEPARATION AND RECOVERY OF METAL IONS

Chem.
Chem. Engr.

Currently, research is being done on both the chemical and chemical engineering aspects of metal ion separation and recovery for the nuclear industry. Projects include the development of solvent extraction process flowsheets for nuclear-waste management. This development will greatly reduce the costs of waste disposal and increase safety by separating radioactive elements from nonradioactive ones. The research uses radioactive tracers and computer modeling, among other methods, to simulate and evaluate potential flowsheets. A participant assisting this group would have the opportunity to learn state-of-the-art techniques in separation science and technology as well as gain practical experience in problem solving.

647 TREATMENT OF SPENT NUCLEAR FUEL

Chem.
Chem. Engr.
Mech. Engr.

Methods are being developed for treatment of spent nuclear fuel for disposal. One of the methods is electrometallurgical treatment, which involves electrorefining the fuel to separate uranium from the fission products. This separation reduces the volume of highly radioactive material that must be placed in a geological repository for disposal. The development work is done with nonradioactive components, which allow hands-on experimental development of the electrorefining process. The electrorefining process is conducted in a high-temperature (500°C) molten salt electrolyte, and it is applicable to a number of other metals beside uranium. A wide range of experimental activities is possible for further development of this technology.

648 TREATMENT OF ELECTROREFINING WASTE

Chem. Engr.
Chem. Engr.
Mech. Engr.

Zeolite, an alumino-silicate mineral that occurs in nature, is being developed as a medium for isolation of radioactive fission products and actinide elements for permanent disposal. The electrometallurgical treatment of spent nuclear fuels results in molten chloride salts having fission products and actinide elements in solution. These salts can be absorbed in zeolite because the zeolite structure has molecular cages that are suitable for accepting a wide variety of anions and cations. In the present research, the salt-loaded zeolite is mixed with glass powder and sintered. The sintering process converts the zeolite to another mineral, sodalite, which has smaller molecular cages. The smaller cage size inhibits release of the salt, actinides, and fission products to the environment. The research opportunities include possible application of this zeolite immobilization technology to other types of radioactive or hazardous wastes.

BATTERY RESEARCH AND DEVELOPMENT

649 BATTERY MATERIALS RESEARCH AND DEVELOPMENT

Ceram. Engr.
Chem.
Chem. Engr.

Novel oxide, nitride, sulfide, salt, and metal alloy materials are being developed and/or modified for use in advanced battery electrodes to improve their performance and life. The research involves the chemical synthesis and processing of these materials and subsequent structural, physical, chemical, and electrochemical characterization. Major equipment includes: X-ray diffractometer, scanning electron microscope, neutron diffractometer, inert atmosphere gloveboxes, furnaces, thermogravimetric and differential thermal analyzers, particle size analyzer, dilatometer, and porosity analyzer.

Mat. Sci.

650 ELECTROCHEMICAL RESEARCH ON ADVANCED BATTERIES

Chem. Engr.
Chem. Engr.
Elec. Engr.

Electrochemical research is being conducted on advanced battery systems, such as Li-polymer and Li-ion.. The purpose of this effort is to understand the fundamental electrochemical phenomena in these advanced batteries and identify the processes and/or components that limit cell performance. In these investigations, laboratory cells are built and characterized by a wide variety of electrochemical techniques. Major equipment includes: data acquisition and control systems, potentiostats/galvanostats, AC impedance analyzers, calorimeters, computers, oscilloscopes, and battery cyclers.

Mech. Engr.

651 MODELING AND DESIGN OF ADVANCED BATTERY SYSTEMS

Chem. Engr.
Elec. Engr.
Mech. Engr.

Modeling and design studies are being conducted on advanced battery systems. In this work algebraic and differential equations describing physicochemical phenomena are developed and solved numerically to characterize and predict cell and battery performance. Fundamental electrochemical transport models on individual cells are developed to fully understand cell performance and add support to the experimental research effort. This work is combined with a relatively applied modeling and design effort to predict the optimum performance of full-sized cells and battery packs.

HAZARDOUS WASTE

652 APPLICATION OF BIOREMEDIATION TECHNOLOGIES TO ACTINIDE CONTAMINATION IN GROUNDWATER

Chem.
Chem. Engr.
Envr. Engr.
Micro biol.

The focus of this research is to investigate the interactions of multivalent actinides with microorganisms under environmentally relevant conditions. In this work the effect of actinides and actinide-chelate complexes on the biodegradation of organic substrates and the impact that biological processes have on actinide redox and chemical speciation are being studied. Current emphasis is on the interaction of Pu, Np, and U with a variety of aerobic and anaerobic bacteria in pure and mixed culture. This research utilizes high-sensitivity spectroscopic methods (X-ray absorption near edge spectroscopy, X-ray absorption fine structure spectroscopy, laser photoacoustic spectroscopy, and laser-induced fluorescence), electrochemical/potentiometric methods, conventional microbiological techniques, and radiometric counting methods. The goals of this research are to develop bioremediation strategies to clean up sites contaminated with actinides and organic wastes and to help assess the role that microbial activity plays in affecting actinide transport in subsurface systems.

653 APPLICATION OF AQUEOUS BIPHASIC EXTRACTION TO RADIOACTIVE WASTE TREATMENT

Chem.
Chem. Engr.
Envr. Sci.

Aqueous biphasic extraction involves the selective partitioning of either solutes or colloid-size particles between two immiscible aqueous phases. Wet grinding of radioactive residues to an average size of one micron will be used to liberate actinides from the bulk of the particle matrix. The processing goal is to produce an actinide concentrate that will more effectively integrate with existing and developing chemical recovery processes.

BASIC AND APPLIED RESEARCH

654 INTERFACIAL MATERIALS CHEMISTRY

Ceram.
Chem.
Chem. Engr.
Mat. Sci.

In this program, advanced spectroscopic techniques (infrared, electronic absorption, nuclear magnetic resonance, and Raman spectroscopy) are used to investigate the catalytic and structural properties of molecular-sieve materials. The emphasis of the research is directed mainly at the mechanisms of catalysis that lead to NO_x reduction, CH_x oxidation, and carbon-hydrogen bond activation. Molecular sieves with intermediate pore sizes and molecular clusters incorporated in large pore sieves are primary focal points in this effort. Major equipment includes: Raman, visible, infrared, and NMR spectrometers; scanning Auger/XPS (X-ray photoelectron spectroscopy) instrument; scanning electron microscope with X-ray analyzer; and gas chromatographs.

655 FLUID CATALYSIS

Chem. Chem. Engr. Mat. Sci. Phy.

Homogeneous and heterogeneous catalysis chemistry and mechanisms associated with the activation of methane, dihydrogen, carbon dioxide, carbon monoxide, and dinitrogen are explored using *in-situ* spectroscopic and kinetic techniques. Parallel synthetic efforts are directed toward the isolation or synthesis of organometallic reaction intermediates and new catalytic species. Catalytic reactions in supercritical fluids and catalytic C-H bond activation chemistry, catalytic formation of pre-ceramic organometallic polymers, and shape-selective macrocyclic catalysts are also investigated. In addition, new high-pressure NMR spectroscopic and NMR imaging techniques are developed to investigate organometallic systems. Major equipment includes: high-pressure multinuclear NMR facility, high-pressure Fourier transform infrared spectroscopy, liquid and gas chromatographs, and high-pressure autoclaves.

656 SPECTROSCOPIC AND SYNCHROTRON STUDIES IN SURFACE AND INTERFACIAL ELECTROCHEMISTRY

Chem. Chem. Engr. Elect. Engr Envr. Sci. Mech. Engr. Metal. Engr. Nucl. Engr. Phy. Mat. Sci. Corr. Sci.

Areas of research are: (1) vibrational spectroscopic, infrared, Raman, and synchrotron X-ray investigations of electro-chemical systems, as well as fundamental studies of the structure of the solid-liquid interface and the nature of the adsorbed state; (2) corrosion and passivation behavior of metals and alloys in various solution environments and as a function of temperature; and (3) deposition processes in boiling and cooling water systems. Electrochemical techniques (e.g., steady-state polarization, cyclic voltammetry, potentiostatic and galvanostatic transients, rotating ring-disc electrode, and AC impedance), spectroscopic methods (e.g., laser Raman, IR, and photocurrent spectroscopies) and synchrotron radiation techniques (X-ray scattering, X-ray absorption spectroscopy, X-ray diffraction, and IR) are employed in the investigations. Major equipment includes: complete electrochemical instrumentation; laser-Raman, and IR spectrometers; high-temperature high-pressure aqueous-corrosion facility; access to the National Synchrotron Light Source at Brookhaven National Laboratory and the Advanced Photon Source at Argonne (X-ray and IR beam lines).

657 THE STUDY OF ELECTROCHEMICAL INTERFACES IMPORTANT TO ENERGY TECHNOLOGIES

Chem. Phy.

The primary objective of this interdisciplinary research is gaining a fundamental understanding of the solid/solution interfacial structure of materials important to energy technologies, particularly energy storage and energy conversion. The problem areas include electrocatalysis, surface morphology of metal deposition/dissolution, under-potential deposition, the intercalation/deintercalation mechanism, and the structure of the electric double layer. The final aim is to contribute seminal guidance to the development of improved energy storage/conversion materials with increased energy and power density and charge/discharge rate for a variety of battery and fuel cell systems, and to improve our understanding of corrosion processes occurring in every energy technology. While we expect that the results of our investigation will provide impetus for technological developments, they will also be of fundamental scientific importance in the field of interfacial electrochemistry. The research program that we carry out couples *in situ* synchrotron-based x-ray measurements (at Argonne's Advanced Photon Source) with electrochemical transient techniques and theoretical modeling.

658 ION TRANSPORT PROPERTIES

Ceram. *Chem.* *Chem. Engr.*

This program uses *in situ* magnetic resonance imaging (MRI) to better define electrode-electrolyte interfaces and solid-state ion transport mechanisms. Areas of interest include the analysis of the chemical composition at the electrode-electrolyte interface, ion concentration gradients within solid-state batteries, conformational dynamics of polymeric electrolytes, and ion penetration depths within graphite insertion electrodes. Special emphasis is placed on measuring ionic diffusion coefficients as a function of distance from the working electrode to probe the mechanism of ion transport in lithium-polymer electrolyte battery materials. Major equipment includes: multinuclear NMR facility, NMR-electrochemical imaging cells, magic angle spinning, Fourier transform infrared spectroscopy, and liquid and gas chromatographs.

659 CHEMISTRY OF SUPERCONDUCTING CERAMICS

Ceram. *Ceram. Engr.* *Chem.*

This research is directed toward the development of alternative processing methods leading to the production of high-quality superconducting ceramics in the Bi-Sr-Ca-Cu-O system. The inorganic chemistry affecting the extent and modes of reaction between the metal oxides will be investigated. Major equipment includes: optical and scanning electron microscopes, differential thermal analyzers, and imaging Raman microscope.

Chem. Engr.

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

660 TRACE-ORGANIC ANALYSIS OF ENERGY AND ENVIRONMENTALLY DERIVED MATERIALS

Chem. *Comp. Sci.* *Envr. Sci.*

A wide variety of chemical carcinogens and toxins with potential health and safety implications are analyzed. Chemicals responsible for hazards are identified and measured. Methods used include gas chromatography (GC), combined gas chromatography/mass spectrometry (GC/MS), high-performance liquid chromatography (HPLC), HPLC/MS, supercritical fluid chromatography (SFC), Fourier transform infrared spectrometry (FTIR), wet chemistry, and computer analysis. In some cases, chemicals present below the parts-per-billion level are detected. Sophisticated computer-controlled analytical equipment is used.

661 METHOD DEVELOPMENT IN TRACE-ORGANIC ANALYSIS

A variety of analytical problems are encountered in trace-organic analysis for which methods are not currently available. Methods are being developed to meet these needs. Recent and ongoing method development examples include PCB and dioxin analysis, air sampling, and stack gas monitoring. Recent instrumentation development includes GC/matrix-isolation/FTIR, multi-dimensional GC, capillary GC, and mass spectrometry. Major equipment includes: GC, SFC, HPLC, MS, MS/MS, and FTIR.

662 MODERN METHODS FOR TRACE ELEMENT ANALYSIS

Chem. Analy. Chem. Analy. Methods Chem. Anal. Envr. Chem.

Improved analytical methods are being developed, evaluated, and implemented for the determination of trace elements in a broad range of sample matrices, including soils, sludges, coals, solid and liquid wastes, and waters. Projects involve both conventional and nonconventional sample preparation methods, separations, and state-of-the-art instrumental analysis techniques. Sample preparation schemes can utilize conventional dissolution techniques, more modern dissolution techniques such as microwave digestion procedures, or less common dissolution techniques employing bomb combustions for the destruction of organic matrices. Separations include both batch and column techniques. Instrumentation available for these projects includes: atomic absorption spectrophotometers (flame, graphite furnace, hydride generation, and cold vapor), an inductively coupled plasma/atomic emission spectrometer, an inductively coupled plasma/mass spectrometer, and an ion chromatograph.

663 TRACE ELEMENT SPECIATION

Proc. Chem. Analy. Chem. Bio-chem. Envr. Sci. Geol. Sci.

The equilibria between organic and inorganic species frequently regulate trace element chemistry. Understanding this chemistry is often critical in studies of biochemical, geochemical, or industrial processes. Current research is directed toward the accurate and sensitive determination of trace inorganic and organometallic species in various media, with an eye toward understanding the relationship between chemical speciation and parameters such as oxidation state, chelation, solubility, and bioavailability. In particular, liquid chromatographic methods coupled with atomic spectrometry (atomic emission or plasma source mass spectrometry) are being developed and used to study relevant equilibria; however, other quantitative techniques and/or structural analysis techniques are within the scope of this work. Elements of particular interest include: chromium, arsenic, selenium, technetium, tin, iodine, mercury, lead, uranium, and plutonium.

664 DETERMINATION OF LONG-LIVED ACTINIDES IN ENVIRONMENTAL MEDIA

Chem. Analy. Chem. Envr. Sci.

Procedures have been developed to efficiently determine the amount of small (10^{-12} Ci) quantities of radionuclides such as plutonium and uranium in soil, water, and other environmental media. It is necessary to characterize large numbers of DOE sites not only to assess contamination levels for subsequent treatment but to determine sites that can be safely released to the public. The actinides are determined using alpha-pulse analysis after dissolution and chemical separations.

665 ASSESSMENT OF DATA QUALITY AND LABORATORY PERFORMANCE IN EVALUATION PROGRAMS

Math.
Comp. Sci.
Envr. Sci.
Analy. Chem.

The Argonne Analytical Chemistry Laboratory collects data from performance evaluation (PE) programs administered by DOE and the Environmental Protection Agency for laboratories providing analytical services to DOE. These data are collected electronically and then analyzed using statistical treatments that allow further assessment than that provided by the base program, such as historical trending and current assessments across multiple PE programs. These treatments of the data allow us to better understand the quality of data generated by a laboratory and to assess how well an individual laboratory is performing. Information about optimizing methods for use in environmental analysis can also be derived from these data.

CHEMISTRY DIVISION (CHM)

The areas of investigation in this Division include chemical sciences and materials science research. Chemical sciences research covers such areas as radiation chemistry, photosynthesis, theoretical chemistry, metal-cluster chemistry, intermolecular dynamics and chemical kinetics, separations chemistry, coal chemistry, and chemistry of the actinide elements. In materials science, the research concerns the chemistry of surfaces and interfaces, the preparation and characterization of organic conductors and superconductors, and structural studies of materials important to energy technologies.

666 RADIATION CHEMISTRY AND PHOTOCHEMISTRY

Chem.
Phy.
Bio.

Chemistry induced by ionizing radiation is studied utilizing state-of-the-art accelerators and lasers. The identity and dynamics of transient intermediates produced by pulse radiolysis or laser photoionization are examined to learn about the mechanisms of energy deposition, transformation, and transport in condensed media. Current studies include experimental and theoretical studies of electron solvation and reactivity, radical cation transformations and reactions in condensed phase, studies of H atoms, charge-pair dynamics, and excited states in photoionization and radiolysis. Radiation Chemistry studies in supercritical fluids (CO_2 and water) examine reactivity of transients. Parallel studies of radical ions are carried out in low-temperature matrix systems. New matrix isolation methods utilize zeolites to control radical-ion reactions and transformations. Appropriate techniques are used to study real-time behavior of transient species. Femtosecond, picosecond and nanosecond absorption and emission studies are carried out with pulse-probe, streak camera, and photon-counting methods. Studies in the nanosecond time domain include dc-conductivity, optical, and special time-domain magnetic resonance methods.

These studies have broad relevance to many fundamental problems in chemical reactivity, to radiation-induced polymer modification, zeolite catalysis, and to the understanding of biological effects of ionizing radiation. A significant challenge is to provide the knowledge base needed to guide the technological development necessary for storage of the radioactive waste forms.

667 PHOTOSYNTHESIS: THE PRIMARY EVENTS LEADING TO STABILIZED CHARGE SEPARATION AND ASSOCIATED MOLECULAR STRUCTURES

Bio-chem.
Bio-phy.
Chem.

The photosynthesis research begins with the growth of photosynthetic organisms (algae and bacteria) and extends to experimental investigations of how light is converted to useful chemical energy, i.e., separation of charge. These investigations emphasize the kinetics and associated molecular structures involved in the initial light-induced chemical reactions of photosynthesis. Photosynthetic reaction center are isolated and probed by advanced spectroscopic techniques, including electron paramagnetic resonance (continuous wave and pulsed), time-resolved electron paramagnetic resonance, time-resolved optical spectroscopy, small-angle neutron scattering, light scattering, and mass spectroscopy. All experiments are under computer control. In addition to the natural photosynthetic systems, model systems such as derivatized small semiconductor colloidal particles are also studied. Fundamental interpretation of the experimental results utilizes theoretical modeling of photosynthesis and/or magnetic resonance that is conducted with a large variety of computers.

668 MOLECULAR PHOTONICS RESEARCH

Chem. *Phy.* The development of molecular electronic devices that use light is a rapidly growing enterprise that seeks to use molecules as electronic switches, wires, microsensors for chemical analysis, and opto-electronic components for use in optical computing. The principal advantages of using molecules in these applications are high component density, increased response speeds, and high energy efficiency. The goals of this research project are to (1) synthesize ultrafast molecular switches based on reversible electron-transfer reactions, (2) investigate the optical switching properties of these molecules using femtosecond optical spectroscopic techniques, (3) characterize thin polymer films of these switching molecules, (4) develop methods to incorporate these molecular switches into conductive polymers, (5) develop methods to incorporate these molecular switches into ordered polymers and self-assembled monolayers, (6) characterize the fast-switching capabilities of these materials, and (7) construct and characterize modulators, holographic memories, and unique optical processors based on molecules.

669 CHARACTERIZATION OF MACROMOLECULES BY MASS SPECTROMETRIC TECHNIQUES

Chem. The objective of this study is to characterize large molecules derived from fossil materials such as coals, kerogens, and petroleum, and from biomacromolecules. Soft ionization techniques such as low-voltage electron impact and fast atom bombardment create the ions, followed by high-resolution mass spectrometry and tandem mass spectrometry to identify the ions formed. Other approaches used include pyrolysis gas chromatography mass spectrometry and laser desorption time-of-flight mass spectrometry. Projects vary from instrument development applications in energy research.

670 NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY

Chem. The Chemistry Division NMR Laboratory is involved in multidisciplinary areas of research, with its primary focus on structure elucidation of complex proteins, organic superconductors, organic extractants, fossil fuels, catalysts, and biomimetic systems. The program consists of the following areas of research: 2-D NMR studies of complex molecules; routine NMR analyses; solid-state NMR spectroscopy of polymers, fossil fuels, and catalysts; and 3-D NMR imaging of materials. The NMR Laboratory is equipped with five state-of-the-art superconducting NMR systems ranging in field strength from 11.7 Tesla (500 MHz proton frequency) to 2.3 Tesla (100 MHz proton frequency). Excellent computing facilities are also available within the NMR Laboratory.

671 MAGNETIC RESONANCE IMAGING

Chem. The magnetic resonance imaging (MRI) program is concerned with the development of new MRI strategies for performing three-dimensional chemical analyses in solving a wide range of problems of current interest. The approach involves the use of advanced computer-controlled nuclear magnetic resonance (NMR) instrumentation for image acquisition, image display, and complete three-dimensional visualization data. Imaging techniques are being applied toward elucidating microchemistry and properties of advanced polymer blends and composite materials, in mapping complex flow patterns of penetrants and pollutants through the soil flushing horizons for environmental restoration and in monitoring solvent diffusion within polymers to probe molecular architecture.

672 CATALYSIS: SYNTHESIS OF NEW MATERIALS

Chem. Two current national concerns are the development of cleaner energy sources and the extension of our own energy reserves. Both of these issues can be addressed by research into new catalysts. The specific project in our group involves the synthesis and characterization of new catalysts that are designed to be used for hydrocarbon processing by the oil industry. The nature of this work combines aspects of inorganic chemistry, geochemistry, and physical chemistry. Experiments involve bench-scale preparation of these inorganic catalysts using inorganic solid-state techniques. The silicates and other oxides are prepared from aqueous solutions treated at high temperature and pressure. Characterization is accomplished by thermal analysis methods, X-ray powder diffraction, surface area measurements, and UV-visible spectroscopy. Interestingly, the materials we make as catalysts can also be used as reinforced nanocomposites, and so some work in the project may deal with this aspect.

673 COAL GEOCHEMISTRY

Chem. Understanding the processes by which organic materials are transformed, under geologic conditions, into coal and oil ultimately helps us to better understand the structure and
Geo. hence, the reactivity of these materials. In this program, we are studying geochemical
Chem. transformations in a number of natural plant biopolymers that are relevant to coal structure. Both the modern biopolymers (e.g., lignin, sporopollenin, and plant resins) and their coalified products (vitrinite, sporinite, and amber) are being isolated and characterized using a wide variety of organic chemical procedures and instrumental analyses (e.g., GC-MS, high resolution-MS, MS-MS, FTIR, and solid and liquid NMR). This project offers the opportunity to acquire and apply practical knowledge of organic chemistry to the characterization of a variety of modern and coalified natural products.

674 BATTERY CARBONS

Chem.
Electro chem.
Mat. Sci.

The need for rechargeable high energy power sources has lead into a new era of research and development in the battery field. Lithium secondary (or lithium ion) batteries are among the energy systems of the future because of their low density, high energy capacity, and long cyclibility. Our group is involved in the synthesis and characterization of novel carbon materials used as anodes in lithium ion cells. Inorganic templates and a variety of organic precursors in liquid and vapor phase are used to produce these carbons. A number of techniques are employed for the chemical and electrochemical characterization: cyclic voltammetry, impedance spectroscopy, galvanostatic control, thermal analysis methods, X-ray power diffraction, surface area measurements, scanning electron microscopy, transmission electron microscopy, and x-ray and neutron scattering techniques.

675 THEORETICAL CHEMISTRY

Chem.
Comp Sci.
Math.
Phy.

The theoretical chemistry program includes studies of the energetics and dynamics of chemical reactions, the nonlinear dynamics of intramolecular energy transfer, and the structure and spectra of molecules. Current research areas include studies of elementary chemical reactions involved in the oxidation of hydrocarbon species. This area involves the use of large-scale computers with emphasis on parallel computing.

676 SEPARATION AND CHARACTERIZATION OF COAL MACERALS

Chem.
Phy.

Coal macerals are coalified ancient plant remains that make up the organic portion of coal and can still be microscopically identified. This program is concerned with the study of the separation and characterization of the macerals to provide more selective feed-stocks for various processes. The project is basic-research oriented and involves some methods of separation similar to those used to separate cells and cellular components. Various methods are used to characterize the macerals, including density gradient analysis, microscopic analysis, Fourier-transform infrared spectroscopy, swelling properties, elemental analysis, and molecular affinity.

677 EXPERIMENTAL METAL CLUSTER CHEMISTRY

Chem.
Phy.

The chemical and physical properties of clusters of metal atoms, such as Fe, Co, Ni, Cu, Al, Cr, V, and Nb, are under study. Chemical reactions are carried out in a laser-vaporization cluster source coupled to a continuous-flow reactor and followed by laser ionization time-of-flight mass spectroscopy to determine product compositions. Studies of reaction kinetics, thermodynamics, catalysis, and cluster structure are being pursued. Physical properties such as cluster ionization potentials and cluster-adsorbate infrared spectra are measured by photoionization, photodissociation, and resonantly enhanced ionization techniques.

678 CHEMICAL KINETICS

Chem. This program involves the study of reactive processes of small radicals in shock tubes. Two different shock tubes are in operation. In one, flash photolysis or excimer-laser
Phy. photolysis is used to create radicals in the shock-heated gas mixture, and the decay or formation of the atomic products is followed by atomic resonance absorption spectroscopy. In the other, the concentration of radicals in high-temperature gases immediately behind the shock front is detected by a pulse of tunable, vacuum-ultraviolet laser light created by nonlinear four-wave mixing in mercury vapor. Current research areas for both shock tube studies focus on chemical reactions involved in the oxidation of hydrocarbon species.

679 THEORETICAL AND COMPUTATIONAL STUDIES OF ATOMIC CLUSTERS

Theor. Chem. Theoretical studies of chemical and physical properties of atomic clusters are carried out. These include investigation of structural, dynamical, and electronic features of clusters, such as geometries, isomerization and phase-change transitions, fragmentation, ionization
Theor. Phy. potentials, electron affinities, chemical reactivity, etc. Both analytical and numerical (computer) simulation techniques are used. The work involves development of new fundamental concepts and theoretical techniques specifically tailored for application to
Math. finite systems.

Comp. Sci.

680 VACUUM ULTRAVIOLET LASER STUDIES

Chem. A vacuum ultraviolet laser system for high resolution photoionization studies of atoms and transient species in gas phase is being implemented and enhanced. VUV coherent
Phy. light is generated by THG, SFG and other suitable methods. The pulsed nature of the laser system enables studies of highly reactive species whose effective lifetime is too short for study by conventional means. The target ephemeral species for study by photoionization are produced in pulsed and CW molecular beams by various *in situ* techniques, such as photodissociation, chemical reactions, pyrolysis, etc. The versatile design of the apparatus allows the application of sophisticated photoionization techniques such as ZEKE, MATI, PEPICO, and others.

681 PHOTOIONIZATION RESEARCH OF RADICALS IN GAS PHASE

Chem. A state-of-the-art photoionization mass spectrometer is adapted to the study of transient species involved in combustion, atmospheric chemistry, and industrially important
Phy. chemical processes. The species of interest are generated *in situ* by various suitable techniques, such as chemical abstraction reactions, electric and microwave discharges, pyrolysis, on-line synthesis, laser photodissociation, etc. The study of threshold and resonant phenomena produces new and significant spectroscopic insights on these ephemeral species. Energy thresholds, such as ionization potentials and fragment appearance potentials, are being determined with high precision and subsequently used to derive useful thermodynamic quantities, such as bond energies and heats of formation. These studies produce novel insights into chemical bonding patterns and unravel systematic behavior in the autoionization phenomena. The stream of forefront data produced by these experiments puts to test the accuracy and predictive ability of the most sophisticated *ab initio* calculations and provides a constant impetus for further theoretical developments.

682 PREPARATION OF ORGANIC EXTRACTANTS FOR METAL VALUE RECOVERY

Chem. New chelating agents soluble in organic solvents (which we call extractants) are synthesized using both standard literature procedures and novel synthesis techniques. Our principle emphasis is on organophosphorus compounds and cyclic polyethers. The principal target metal ions are those of importance in the handling and management of radioactive materials. The new compounds are purified using standard techniques, including gas and liquid chromatography. Characterization of the compounds is accomplished using standard spectroscopic techniques like NMR, IR, and mass spectrometry. These new compounds are then evaluated for their potential application in metal ion separations..

683 APPLICATION OF LIQUID-LIQUID EXTRACTION AND EXTRACTION CHROMATOGRAPHY TO METAL ION SEPARATIONS

Chem. Solvent extraction reagents, are examined for their potential application to metal ion separation problems. Our primary emphasis is on the development of new procedures for the handling and processing of radioactive materials (actinides, cesium, strontium, other fission products, actinide decay daughter products). A secondary interest is in developing new separation systems for commercially and strategically important metal ions. The characterization consists of determination of the extraction efficiency and selectivity of new reagents, their physical behavior toward the target ions and potential interfering species, and the ease of recovery of extracted metal ions. A wide variety of analytical techniques (for example, radiochemistry, spectroscopy, X-ray and neutron scattering techniques) are applied in the characterization of these new materials.

684 LASER DESORPTION/IONIZATION MASS SPECTROMETRY

Chem.
Comp. Sci.
Phy.

Mass spectrometry of organic molecules and biomolecules is explored using digital computer-aided time-of-flight mass spectrometry lasers. This method has analogs in FAB, ^{252}Cf-PDMS, and secondary-ion mass spectrometry. Laser desorption is used to analyze high-molecular-weight compounds that are important to geochemical samples, such as coals and petroleum products. Studies of the particle-induced desorption process are being undertaken to provide insight into the mechanisms of ion and neutral desorption. Participation in this research affords the opportunity to become acquainted with state-of-the-art mass spectrometric methods.

685 NOVEL ORGANIC CONDUCTORS AND SUPERCONDUCTORS

Chem.
Mat. Sci.
Phy.

New organic conductors and superconductors, which have novel electrical and magnetic properties, are synthesized and then characterized by use of various techniques. The organic donor and acceptor molecules are prepared in our laboratories and the conducting salts are grown with the use of simple electrocrystallization techniques. Projects in this area of research include organic and inorganic synthesis; crystal growth using a variety of techniques; compound characterization by use of IR, and NMR; structural characterization using X-ray diffraction (state-of-the-art Siemens “SMART” Area Detector System) and computer analysis of results; electrical conductivity and superconductivity measurements; variable-temperature electron-spin resonance spectroscopy; magnetic susceptibility studies (1.6 - 300 K); Raman spectroscopy.

686 CONDUCTIVE ORGANIC THIN FILMS

Chem.
Mat. Sci.
Phy.

This project, which is closely related to project "Novel Organic Conductors and Superconductors", is centered around the fabrication and characterization of thin conducting films composed of organic molecules. Thin films of these unusual materials are especially suitable for their eventual application, e.g., in chemical sensors or electronic devices. Electrochemical and chemical techniques are employed to prepare the charge transfer organic thin films. Infrared, Raman, and UV-Vis spectroscopies, x-ray diffraction, scanning probe microscopy, conductivity measurements, etc., will be used to characterize the structural and physical properties of these thin films.

687 SURFACE AND INTERFACIAL CHEMISTRY

Chem.
Metal. Sci.
Metal. Engr.
Phy.

Exemplified by the increasingly stringent demands of the electronic industry for unambiguous quantitative identification of trace impurities in semiconductor materials at high lateral resolution and by the environmental need for isotopic and elemental analysis of micron sized grains, trace analysis on samples of atomic dimensions has become an important analytical problem. Resonance Ionization Mass Spectrometers (RIMS) have been developed that combine both high sensitivity and high discrimination allowing for the first time trace analysis of samples with impurity atom counts of only a few hundred - even when the impurity concentration is below 100 ppt. Additional benefits of the instrumentation are discrimination from isobaric impurities and an ability to make measurements in regions of changing chemical compositions.

These RIMS instruments are being applied to a wide range of fundamental and applied surface science problems. Presently under investigation are (1) the fundamentals of energetic ion and laser - solid interactions, (2) ultra-trace semiconductor impurity analysis, (3) ways of improving plastics by understanding additive surface diffusion, (3) anodic film formation in Mg electrowinning, and (4) isotopic analysis of meteorite grains.

PHYSICS AND CHEMISTRY OF HEAVY ELEMENTS

This section is concerned primarily with the chemistry of lanthanide and actinide elements.

688 ACTINIDE AND LANTHANIDE COORDINATING CHEMISTRY

Chem.
Radio-chem.
Coor. Chem.

Lanthanides and actinides (f elements) are unique in the periodic table, being the only elements having valence electrons in f orbitals. The lanthanides are important in a variety of material science applications (and increasingly in medicine, for example, as magnetic resonance imaging agents) while the actinides (almost all man-made) are the elements necessary for nuclear power. This program is devoted to the investigation of the physical chemistry of the formation and dissociation of f element complexes with chelating organic ligands, and to the determination of the structural features of such complexes. One additional goal is to elucidate guiding principles for the design of new chelating agents of general utility using the unique properties of f elements. Results obtained from investigations of the fundamental chemistry of actinides are used to develop new technologies for improved separation/isolation and environment restoration options. Our facilities include laboratories designed for work with radioactive materials, NMR spectrometers, single crystal and powder diffractometers, fast-kinetics (stopped-flow/T-jump) spectrophotometer, potentiometric titration laboratory, calorimetry laboratory, and an organic synthesis laboratory with complete instrumentation. The principal focus is on solution chemistry, but other methods/media are investigated as required.

689 SOLID-STATE ACTINIDE CHEMISTRY

Chem.
Mat. Sci.

Systematic studies that focus on the cooperative interactions of f electrons in solids are the theme of this research effort. A program involving the determination of magnetic and superconducting properties of ceramic oxides, and how these properties are influenced by structure, is now well established. This topic has received considerable publicity since superconductivity was observed to occur at 90° K in a subclass of these oxides. Structural problems are solved with state-of-the-art X-ray diffraction, or pulsed-neutron diffraction facilities; the latter in collaboration with scientists at Argonne's Intense Pulsed Neutron Source. In-depth investigations of magnetic properties of well-characterized materials are done with a modified Faraday magnetometer coupled to an IBM-PC, with extensive data interpretation handled on IBM or VAX mainframes. Although this is a basic research effort, applications in such diverse areas as waste management of radioactive elements or technological uses of high-T_c superconductors are spin-offs of this research.

690 PHOTOCHEMISTRY AND PHOTOPHYSICS OF HEAVY ELEMENTS

Chem.
Phy.
Photo-chem.

The chemical and physical consequences of creating excited electronic states unique to f elements are being investigated in gas, liquid, and solid phases. This research effort is defining the forefront of fundamental photophysics and photochemistry studies of transuranic compounds and exploits lanthanide analogs in comparing the behavior of 4f and 5f electron systems. We seek a predictive understanding of the excited-state behavior of these systems using high-resolution laser excitation on nanosecond and picosecond time-scales. Time- and wavelength-resolved fluorescence excitation and emission studies from the ultraviolet to the midinfrared are carried out by using computer-controlled digital data acquisition and signal-averaging systems. Investigations of nonfluorescent systems are carried out by means of thermal lensing and photoacoustic spectroscopies. These studies impact the scientific basis of nuclear waste management and efforts to employ photochemistry to efficiently separate actinide elements and isotopes.

691 LASER SPECTROSCOPY OF HEAVIER ELEMENTS IN SOLIDS

Chem.
Phy.

The lanthanides and actinides are unique in the extent to which important aspects of their electronic structure can be deduced from measurements of the absorption and fluorescence spectra of their compounds. Electronic transitions within the 4f states of a lanthanide ion and the 5f states of an actinide ion yield sharp band structures. Experimental and theoretical studies of these transitions provide fundamental understanding of the electronic properties of these heavy elements in crystals and glasses. These studies are essential for improving optical performance of the widely used lanthanide-activated solid state laser materials and for developing new generation of laser optical materials. The studies of actinide materials also impact the scientific basis of nuclear waste management. Opportunity is provided to become acquainted with the high-resolution and non-linear laser spectroscopic techniques used to obtained ion-site resolved spectra, as well as the theoretical models used to interpret these spectra in terms of electronic and nuclear interactions. Particularly, optically-detected nuclear magnetic resonance (ODNMR) is one of the advanced techniques that enable us to overcome inhomogeneous line broadening and to measure the nuclear spin energy levels of lanthanides and actinides in structure-disordered solids. Time-resolved excitation and time-domain measurements are also performed to study the excited-state dynamics of the heavy elements in various compounds. Our laser spectroscopy laboratory is well-equipped for conducting experiments with lasers tunable from IR to UV region and cryostats at temperature controllable from 300 K down to 1.6 K and magnetic field up to 5 tesla.

EXPERIMENTAL ATOMIC AND MOLECULAR PHYSICS

The experimental atomic and molecular physics research in the Chemistry Division is centered around four main programs.

692 ACCELERATOR-BASED ATOMIC PHYSICS

Phy. Details of atomic structure and dynamics are studied using accelerated ion beams from ATLAS (Argonne Tandem Linac Accelerator System). A wide variety of ions can be accelerated to velocities of v/c = 0.1, allowing the study of few electron systems by beam-foil spectroscopy. For example, ultra-short atomic lifetimes (100 fs to 10ps) are being measured by a recently-developed two-foil technique. The first foil is used to excite the ion and the second foil is translated downstream to probe the excited state population. As an example of collisional studies, the multiple fragmentation of C_{60} by highly-charged Xe ions has enabled the study of excitation and decay processes of this molecule at energies exceeding those used in previous work by several orders of magnitude.

693 SYNCHROTRON-BASED ATOMIC PHYSICS

Phy. A new program aimed at utilizing the unique features of the Advanced Photon Source (APS) to probe atomic structure and dynamics has been initiated. The emphasis is on using the high brilliance, high energy photons (E = 40 keV) to study inner shell electrons of heavy and medium-heavy atoms. The X-ray photons are particularly suited to probing correlation, relativity and quantum electrodynamics in many-electron systems. Currently, development of the undulator and monochromator is underway as part of the APS construction in addition to the design of specific equipment for the atomic physics experiments.

694 ION-PHOTON INTERACTIONS

Phy. Measurements are made on interactions involving intersecting beams of fast ions from an accelerator and photons from an intense tunable laser. The project has a variety of objectives; e.g., the laser spectroscopy of exotic ionic species, studies on collisional excitation (in foils or gases) from non-ground-state atomic species, and precision decay time measurements.

695 ACCELERATOR-BASED ATOMIC PHYSICS

Phy. Atomic physics studies are underway at ATLAS, Argonne's heavy-ion accelerator that is capable of generating intense high-quality beams of a wide variety of atomic ions with energies variable up to about 10 MeV/nucleon. X-ray, optical, and electron spectroscopic studies on highly-ionized species are conducted as well as a wide range of other atomic physics research. Precision measurements are being made on radiation emitted by highly-stripped 2- and 3-electron ions to test fundamental calculations of relativistic quantum mechanics.

The 150-kV Blase accelerator produces lower-velocity ions for high-resolution laser-fluorescence and laser rf double-resonance studies of atomic ions. The goals are better understanding of hyperfine structure and relativistic atomic structure.

DECISION AND INFORMATION SCIENCES DIVISION (DIS)

The Decision and Information Sciences Division is composed of several sections that focus their research activities in distinct but related technical areas. The mission of the Division is to develop and apply innovative approaches to resolving matters of national concern related to information management and energy.

MULTIPURPOSE ANALYTICAL TOOLS

The integrated assessments prepared by the Division frequently lead to development of analytical tools and methodologies that can be applied to a wide range of problems.

696 ADVANCED COMPUTING APPLICATIONS

Comp. Engr.

Comp. Sci.

Decision Theory

Info. Sci.

Operation Research

Artificial Intelligence

Comm./Networks

The Division develops artificial intelligence and expert systems, manages very large databases designed to support scientific and engineering activities, and pursues other applications of computer hardware and software that include:

- Enhanced computer visualization
- Global climate modeling
- Hardware selection/configuration
- Mission planning
- Logistics and mobility planning
- Graphical application development environments
- Networking and communications
- Resource allocations
- Treaty verification data systems
- Internet and web-based information systems
- Geographical information systems
- Models and simulation

697 DECISION ANALYSIS

Comp. Sci.

Envr. Sci.

Indus. Engr.

Mech Engr.

The Division uses decision analysis to support decision making by national and international managers, particularly in the area of program planning. Developing these techniques in computerized form leads to improved productivity, reproducibility, and accuracy. Contained in this area of work are:

- Design analysis for regulatory developments
- Portfolio planning
- Site selection
- Technology evaluation and selection
- Remedial investigations, feasibility studies, and risk analyses
- Systems support for decision making

Nucl. Engr. *Operations Research* *Decision Theory*

698 RISK ASSESSMENT AND RISK MANAGEMENT

Comp. Sci.

Oper. Research

Envr. Engr.

Envr. Sci.

The Division develops risk assessment and management techniques for a variety of programs. The issues addressed relate to risk environmental and health risk management and new ways of meeting regulatory requirements. Activities include:

- Application of computer and decision analysis techniques
- Methods development
- Public risk perception
- Risk communication
- Uncertainty analysis

ENERGY SYSTEM ASSESSMENT

The nation is again focused on the need to address issues of energy supply and demand, to choose appropriate energy technologies, and to develop new and existing energy supplies.

699 ENERGY SUPPLY AND DEMAND ANALYSIS

Bus. Admin.

Econ.

Energy Engr.

Envr. Engr. *Pol. Sci.* *Policy Sci.* *Pub. Admin.* *Intl. Rel.*

The Division develops energy demand projections, evaluates alternative energy supply systems, and evaluates energy and environmental policies bearing on energy development. The group is currently studying:

- Domestic/international energy plans
- Economic/legislative policy analyses
- Energy/environmental systems and policy analysis
- Acid-rain-related issues

700 ENERGY TECHNOLOGY ASSESSMENT

Bus. Admin.

Chem. Engr.

Econ.

Envr. Engr.

Envr. Sci.

The Division evaluates the technical performance and economics of energy systems, studies the market penetration of energy technologies, and assesses environmental impacts. Areas of interest include:

- Air pollutants, including oxidants
- Clean coal technology
- Control technology evaluation
- Emissions models and databases
- Integrated model development
- Market penetration of energy technologies
- System economics
- Technology assessments

701 EMERGENCY AND CONTINGENCY PLANNING

Bio.
Bus. Admin.
Chem.
Emerg. Plan.
Pub. Admin.

The Division has considerable expertise in emergency preparedness and planning for technology-related accidents and other emergencies. It plans and develops guidance for responding to accidents and other emergencies. It plans and develops guidance for responding to accidents at nuclear and hazardous materials facilities and for related transportation operations. Among topics currently under consideration are:

- Chemical weapon demilitarization
- Energy security
- Hazardous materials
- Infrastructure assurance
- Consequence management
- Technology transfer
- Emergency preparedness
- Radiological emergency preparedness
- American Indian emergency preparedness

THE MINORITY ENERGY RESEARCH PROGRAM

The Minority Energy Research Program, managed by Argonne National Laboratory for the Office of Minority Economic Impact of the United States Department of Energy, is concerned with conducting research that will help the Secretary of the Department design and implement programs that will assist minority energy consumers and minority owners of energy businesses. The key objectives of the Program are: (1) to assemble and analyze a comprehensive database concerning minority energy consumption and expenditures, (2) to advise the Secretary on the impact of energy policy and programs on minority energy use and expenditures, and (3) to conduct research that will aid minority-owned energy business.

702 MINORITY IMPACT - DATA ANALYSIS

Comp. Sci.
Econ.

Work in this project involves assembling, analyzing, and integrating a diverse set of transportation and residential energy databases that can subsequently be used in impact assessments. Present emphasis is on statistical analysis and on identifying statistical tools that will facilitate more integrated use of diverse databases.

Soc. Stat.

703 MINORITY IMPACT - IMPACT ASSESSMENT

Pol. Sci.

This project identifies energy issues of greatest relevance to minority groups and assesses the impact of energy policy and programs on those groups.

Soc. Geog. Urban Planners Econ.

704 MINORITY IMPACT - BUSINESS ASSISTANCE

Finan.
Mktg.

This group works to identify issues of greatest concern to minority owners of small energy-related businesses, and conceptualize connections between them and minority energy consumers.

Urban Planners

ELECTRONICS AND COMPUTING TECHNOLOGIES DIVISION (ECT)

The Electronics and Computing Technologies Division (ECT) is committed to the introduction and provision of the electronics, computing and communications infrastructure to enhance the productivity of and provide new capabilities for the Laboratory's administrative, scientific and engineering programs. The primary goal of ECT is to establish and promote a seamless environment where individual researchers and workers can easily access and use all elements of the ANL information resources hierarchy, independent of the diverse computer, electronics, and telecommunications technologies they choose to use.

705 SYSTEMS MANAGEMENT

Comp. Sci. Systems managers manage the performance of high-performance distributed workstations. Other activities include software installation and configuration, testing of new systems, and necessary programming modifications to address special needs.

706 AUTHENTICATION TECHNOLOGIES

Appl. Math The ability to confidently identify network users is a fundamental requirement for distributed applications. Strong authentication enables sharing sensitive data across unsecured networks. Technologies such as LDAP, Kerberos, and public/private keys to

Comp. Sci. provide alternate authentication strategies. Argonne actively works to incorporate technologies into UNIX and Microsoft environments.

707 HIGH-SPEED NETWORKING

Comp. Sci. Scientific computation demands increased data transmission speeds through high-speed networks to enable the transfer of large data files, effective distributed processing, remote visualization capabilities, and other electronic communication. ECT is developing fiber-

Comp. Engr. optic networks with standard protocols to meet these increasing demands. ANL also participates in the planning, development, and operation of several high-speed national networks.

708 LOCAL-AREA NETWORKING

Comp. Sci. Distributed computing plays an increasingly prominent role in both scientific computing and administrative business systems. The distributed environment at ANL can be characterized as networks of Unix scientific workstations and networks of personal

Comp. Engr. computers integrated via a Laboratory-wide network. Ongoing activities include the design and upgrade of these networks, the development of network servers and services, and the provision of a client-server framework for new scientific and administrative network applications.

709 ELECTRONICS ENGINEERING DESIGN SECTION

Elec. Engr. Designs and implements computer- and microcomputer-based real-time systems, real-time applications software, distributed-intelligence networks, and data links. In addition, the Engineering Section designs instrumentation for nuclear reactors, particle accelerators, telemetry systems, and research programs. Calibration services traceable to the National Bureau of Standards are also provided. This section also develops new instruments and techniques for radiation detection and imaging, pulse spectrometry, and nondestructive analysis. Systems are developed for applications in synchrotron-light research, neutron scattering studies, environmental monitoring, and nuclear physics.

710 INFORMATION SYSTEMS

Comp. Sci. Programmer/analysts develop or modify programs, interact with customers, and conduct system tests associated with developing and maintaining the Laboratory's business information systems in a distributed client-server computing and web-based computing environment. Technologies used include Oracle as the primary database engine, PowerBuilder as the primary graphical user interface tool, IIS as the primary web tool, Unix as the primary operating system, with HP and Sun the primary computing platforms and Windows on the desktop.

ENERGY SYSTEMS DIVISION (ES)

The Energy Systems Division (ES) of Argonne National Laboratory conducts research and development efforts in energy production, efficient energy conversion and use, mitigation of the environmental effects associated with producing and using energy, and methods of restoring contaminated and degraded lands to a usable, productive state. The Division concentrates on laboratory research needed to enable a cleaner and more efficient use of energy resources and on field studies pertaining to the wise use and maintenance of environmental and natural resources

The ES Division is organized into three Centers: (1) The Center for Industrial Technology Systems is strongly committed to developing and transferring clean, efficient energy and industry-related environmental technologies into the marketplace to benefit U.S. companies, the feral government, customers, and the general public, (2) The Center for Environmental Restoration Systems develops and performs research, development and demonstration programs to support the complete environmental restoration process, from start to finish, addressing each of the three stages of the process, and to transfer the knowledge and technologies obtained to sponsors and other potential users of that information, and (3) The Center for Transportation Research conducts research to evaluate and develop transportation technology, with emphasis on reducing petroleum-fuel requirements, costs and environmental consequences of transportation systems.

CENTER FOR INDUSTRIAL TECHNOLOGY SYSTEMS

The Center for Industrial Technology Systems acts as national resource in supporting the missions of the U.S. Department of Energy and private industry. The Center is strongly committed to DOE's Office of Industrial Technology in transferring clean, efficient energy technologies into the marketplace to benefit U.S. companies, federal government customers, and the general public.

711 DEVELOPMENT OF ADVANCED ENVIRONMENTAL CONTROL TECHNOLOGY

Chem. Engr. Chem. Engr. Engr. Sci./Engr. Mech. Engr.

The objective of this project is to develop advanced techniques for the control of air emissions from the combustion of fossil fuels. Many of the technologies are also applicable to systems that involve combustion of municipal waste or hazardous chemical wastes. Currently, the project focus is on technologies for the control of mercury emissions, which result from the combustion of coal and several types of waste. Mercury has the potential to cause environmental and human health problems, but it is very difficult to capture since it is usually in the vapor phase at flue-gas temperatures and it is very insoluble in typical flue-gas scrubbing solutions. Laboratory research activities have focused on both advanced types of dry sorbents and techniques for converting elemental mercury into more soluble chemical forms. State-of-the-art laboratory facilities, experimental design and analytical techniques, and computerized data collection/analysis procedures are employed.

712 CHEMICAL AND BIOLOGICAL TECHNOLOGY

Biochem. Engr.
Chem. Engr.
Chem. Engr.
Civil Engr.
Envr. Engr.

This area is focused on integrating chemical engineering with biological processes. A major objective is the development of new methods to produce chemicals utilizing both fermentation and biocatalytic systems, which are integrated with separation and purification technologies utilizing new membrane technologies. Methods to produce a "green" solvent from corn, ethyl lactate, have led to a licensed joint venture and three national awards. Another objective is the development of detection and treatment methods for controlling and understanding sustained localized pitting corrosion influenced by microbes. Other projects include phytoremediation, examining the use of plants for environmental remediation, sonication or advanced oxidation to remediate groundwater and soil, the development and use of new biomodified catalysts, and the use of paleoclimate changes to model hydrocarbon exploration and global warning.

Geol. *Microbio.*

713 FOULING MITIGATION

Chem. Engr.
Mech. Engr.

The overall objective of this program is to conduct applied research in heat and mass transfer. The program focuses on the study of underlying mechanisms in heat and mass transfer enhancements, fouling, and heat and mass transfer in multiphase flow. The research outcome consists of validated models and design methods for high-performance thermal systems. Experimental and analytical work is conducted at Argonne and at supporting subcontractors facilities.

714 CARBON MANAGEMENT

Chem. Engr.
Envr. Engr.
Envr. Sci.
Mech. Engr.

This effort seeks to develop cost-effective, high efficiency, low-greenhouse-gas, and low environmental impact technologies. Ultimately, these technologies will be used in the Utility, Industrial, and Transportation sectors. In cooperation with industry, studies will use full-energy cycle analysis of advanced utility and industrial fossil fuel-based systems to establish base-line greenhouse gas inventories for several current technologies. We are developing a capability to understand and coordinate with groups studying terrestrial and ocean response to natural and anthropogenic induced changes in atmospheric concentrations of greenhouse gases. In addition, we are investigating the development of novel natural gas resources, especially the methane hydrates distributed in ocean sediments throughout the world.

715 PROCESS EVALUATION AND DEVELOPMENT

Chem. Chem. Engr. Envr. Engr. Envr. Sci. Metal. Engr. Metal.

Our focus is on the development of advanced waste minimization/pollution prevention technology, with an emphasis on materials recycling. We have three core activities: (1) physical/chemical separation process development, (2) hydro/pyrometallurgical process development, and (3) process simulation and cost analysis. Representative projects where student help is anticipated include: (1) recovery of materials from auto shredder residue (thermoplastics, polyurethane foams, oxides of iron and silicon for cement-making), (2) recovery and separation of thermoplastics from obsolete appliances, (3) recovery of materials from aluminum salt cake (recovery of salt by electrodialysis, conversion of oxides to value-added products), (4) evaluation of processes for the recovery/recycling of rocket motor chemicals, and (5) evaluation of non-consumable anodes for molten salt electrowinning of metals.

CENTER FOR ENVIRONMENTAL RESTORATION SYSTEMS

The Center for Environmental Restoration Systems performs research, development and demonstration programs to attain all aspects of environmental restoration from start to finish, including site characterization, selection and implementation of remediation technologies for site cleanup, and final restoration of a site to usefulness.

716 GEOLOGIC AND HYDROLOGIC ENGINEERING

Chem. Engr. Civil Engr.

Studies of interaction between energy operations and systems and the environment often involve investigations related to geologic or hydrologic engineering. Current studies deal with development of methods for measuring the effectiveness of site-characterization methods, groundwater modeling, and field measurements associated with environmental compliance at facilities located in diverse settings and locations.

Geol. Geohydrol. Hydrol.

717 RESEARCH AND DEVELOPMENT PROGRAMS TO REMEDIATE CONTAMINATED SITES

Chem. Civil Engr. Chem. Engr. Envr. Engr.

Studies of sites contaminated with hazardous and toxic materials require data acquisition, analyses, and interpretation on many site conditions that determine migration and fate of contaminants. Site properties related to hydrology, soils, geology, geochemistry, and related conditions must be understood to evaluate environmental risks and site cleanup alternatives. Current studies involve environmental geophysics in a range of geologic settings; field investigations of subsurface geology related to contaminant migration; evaluation of the fate of contaminants in soils and uptake of these materials by plants, phytoremediation of soil and plumes, development of standardized analytical chemistry techniques for contaminants; and evaluation of treatment technologies to remediate contaminated soils and groundwater.

718 SPATIAL ANALYSIS AND DECISION SUPPORT SYSTEMS

Geog.
Comp. Sci.
Engr. Design
GIS Special.

Environmental research requires the ability to collect, manipulate, analyze, evaluate, and display data on three-dimensional characteristics and spatial variables at both small and large scales. Geographic information systems (GIS), computer aided design (CAD) software, data base systems frameworks, visual simulation capabilities, remote sensing/satellite imagery collection, and multimedia techniques are used individually and in combination to solve environmental problems. Current studies include global scale simulation of continental drift through geologic time, developing expert systems utilizing input from GIS sources to guide brownfield redevelopment, coupling risk models to GIS, incorporating distributed sensor networks into spatially based decision support tools, and coupling geophysical data to related GIS information.

Remote Sensing Specialist *Landscape Architecture*

CENTER FOR TRANSPORTATION RESEARCH

The Center for Transportation Research (CTR) conducts applied research for the U.S. Department of Energy on advanced transportation technologies and their energy, economic, and environmental impacts. A broad spectrum of technologies are being researched; some examples include alternative-fueled vehicles, magnetically-levitated high-speed vehicles, and environmental impacts of the transportation of hazardous materials. Ongoing work also includes study of energy use and transportation demand under different future scenarios, environmental assessments and modeling of existing and new technologies, and issues and strategies for a transition to alternative fuels. Due to the breadth of current research topics, CTR is interested in attracting both students and faculty from a diverse set of disciplines to contribute to our research efforts.

719 ALTERNATIVE FUELS FOR TRANSPORTATION

Chem. Engr.
Comp. Sci.
Envr. Sci.
Envr. Engr.

CTR is conducting technical, economic, policy, and environmental analyses for a transition to non-petroleum fuels for the transportation system. Projects span light- and heavy-duty vehicles and buses, and include fleet demonstrations. Analysis of alternative transportation fuels in CTR includes: (1) assessment of engine, vehicle, and fuel supply technologies; (2) assessment of the properties of fuels, their combustion products, and atmospheric side effects; (3) econometric analysis of consumer response to the cost changes of fuels and vehicles when adopting alternative fuels; and (4) economic assessment of policies designed to promote the introduction of alternative fuels. Two specified examples of ongoing projects are listed below.

Econ. *Mktg.* *Mech. Engr.* *Pol. Sci.* *Stat.*

720 ALTERNATIVE TRANSPORTATION FUELS - VEHICLE AND FUELS CHARACTERIZATION

Chem. Engr.
Mech. Engr.

This project involves the study of the attributes of engines and fuel systems for various fuels and technologies and develops comparisons of advantages and disadvantages of each. Emissions, energy consumption, power density, and other measures are used as a basis of comparison. Participants in this program may also study fuel-processing and transportation systems such as refineries, pipelines, and ships and may estimate costs of technologies, working with economists.

721 ALTERNATIVE TRANSPORTATION FUELS - ECONOMIC ASSESSMENTS

Econ. Work in this area involves the study of consumer responses to vehicle and fuel characteristics, including price changes and factors such as performance and safety. Policy questions, including issues of short-run costs vs. long-run savings induced by inter-fuel competition are also under investigation Participants in this program will work with engineers to develop cost estimates for new technologies.

722 EXPERIMENTAL DATA COLLECTION

Mech. Engr. A Mechanical Engineering Assistant is needed for acquiring engine test data using high-speed data acquisition system and analyzing the data.

723 ANALYTICAL ENGINEER

Mech. Engr. A Mechanical Engineering or computer systems engineer is needed to conduct simulation studies of engines and vehicle systems.

ENERGY TECHNOLOGY DIVISION (ET)

The Energy Technology Division provides an integrated, state-of-the-art approach to the design, fabrication, and testing of highly-reliable materials, components, and instrumentation. The Division is particularly strong in the areas of high-temperature properties of metals and ceramics, corrosion, radiation effects, nondestructive evaluation techniques, materials processing, thermal hydraulics, engineering mechanics, instrumentation and control, and components and systems testing. For energy technologies, the Division's programs emphasize safe and reliable design, efficient performance, and inherent safety of components and systems, as well as gathering basic engineering data and developing applicable new methods of analysis.

724 INSTRUMENTATION AND NONDESTRUCTIVE EVALUATION

Chem. Engr.
Comp. Sci.
Elec. Engr.
Engr. Phy.
Mech. Engr.
Nucl. Engr.
Phy.

The Instrumentation and Nondestructive Evaluation (NDE) Section conducts research and development in a broad range of energy-related technologies. Major areas of responsibilities are the development of instruments or NDE techniques for fossil energy, conservation, automobile, textile, waste management, and nuclear technologies, as well as for arms control and verification treaties.

The current instrumentation efforts of the Section focus on the development of advanced sensors and control systems. This work encompasses (a) multiphase flow measurement techniques, including in-situ measurement of temperature, fluid level, pressure, density, and viscosity; (b) development of leak detection and location systems for power plants; and (c) a number of projects for arms control to develop sensor/instruments for treaty verification. In addition, work has commenced on smart sensors/systems, photoacoustics and rapid prototyping. Sensors used in the treaty verification project are based on acoustic, microwave/millimeter wave and mass spectrometer techniques.

Our NDE efforts focus on development of techniques and systems for materials characterization and evaluation of component reliability. This work includes (a) characterizing materials, especially ceramics composites, during various stages of fabrication; (b) evaluating the structural integrity of components of a wide variety of energy systems; and (c) pinpointing causes and remedies for improper component behavior through failure analysis. The techniques used to perform this work are based on acoustic, X-ray diffraction and X-ray tomography, NMR spectroscopy and imaging, microwave, neutron diffraction, and optical methods.

725 ANALYTICAL THERMAL HYDRAULIC RESEARCH PROGRAM

Chem. Engr.
Comp. Sci.
Math.
Mech. Engr.
Nucl. Engr.
Phy.

The Analytical Thermal Hydraulic Research Program is responsible for mathematical modeling of thermal hydraulic physical phenomena and for developing computer codes (COMMIX and CAPS series) that can analyze heat transfer and fluid-flow conditions in components of various engineering systems. The computer codes being developed are single-phase/multiphase conservation equations of mass, momentum, and energy. The COMMIX series uses volume porosity surface permeability, distributed resistance, and distributed heat source concepts to analyze continuum/quasi-continuum flow domains. The CAPS code models the flow and solidification of metals in castings and provides a tool for a mold designer to optimize his development work by computer simulation. The COMMIX and CAPS codes have a wide range of applicability and have been successfully used to analyze (1) reactor fuel assemblies (rod bundles), (2) reactor plenum mixing problems, (3) flow stratification problems in a pipe, (4) reactor heat exchangers, (5) reactor steam generators, (6) thermocline storage tanks for solar applications, (7) fluidized-bed combustion processes, (8) rock beds, (9) solar ponds, (10) piping systems and valves, and (11) iron and aluminum casting problems.

726 THERMAL MECHANICAL SCIENCES

Appl. Math.
Chem. Engr.
Civil Engr.
Mech. Engr.
Nucl. Engr.

Research in this group relates to many diverse areas involving structural dynamics, thermal-hydraulics, heat transfer, fluid flow, and vibrations. Program emphasis is placed primarily on experimentation and testing, but also extends to modeling. The group operates several test facilities. These include the Flow-Induced Vibration Test Facility (an 8,000-gpm water flow loop), the Flow and Heat Transfer Test Facility (a computer-controlled, thermal-hydraulic, transient, nonisothermal, 2,200-gpm water loop), a low-velocity water channel, a slurry test facility, an adiabatic two-phase flow apparatus, small-channel flow boiling and condensation heat transfer test apparatus, and a 500-gpm water loop. The group performs fundamental research, component development, and performance testing and consultation. Current activities include research in the areas of flow-induced vibration, multiphase flow and heat transfer in compact heat exchanger geometries, ice-slurries for district cooling, and chaos associated with fluid-structure interaction. In addition, vibration studies are performed in support of accelerator facilities.

727 TRANSPORTATION OF HAZARDOUS MATERIALS

Appl. Math.
Chem. Engr.
Civil Engr.
Comp. Sci.
Mech. Engr.

This group provides technical assistance to the Department of Energy (DOE) by addressing department-wide transportation, traffic, and waste-management options. Generic national and international issues are considered, including packaging certification, transportation tracking systems, related regulations and legislation's, and waste repository configurations. Examples of tasks performed include the review and analysis of DOE-generated reports, the review of scripts for and production of educational and training videos, and the technical review of Safety Analysis Reports for Packagings (SARPs), Waste Facilities Conceptual Design Reports (CDRs), and Final Safety Analysis Reports (FSARs). The SARP reviews involve general information and drawings; structural, thermal, containment, shielding, and criticality analyses; operating procedures; acceptance tests; maintenance programs; and quality-assurance plans. Computer codes are used for analyses. Packaging or facility compliance with DOE orders and federal regulations is ascertained.

Nucl. Engr. *Phy.* *Traffic Management.*

728 CERAMICS

Chem. Ceram. Engr. Mat. Sci. Metal Engr. Mech. Engr.

Ceramic processing development and new ceramic-materials synthesis for a wide variety of applications are carried out in this section. Much of the work is done on a collaborative basis with other groups both within and outside of Argonne. An example is the conductor development using high-T_C ceramic superconductors. The Ceramics Section staff have fabricated wires and other technologically useful shapes for motors, bearings, sensors, etc. as well as synthesized new superconducting compounds. Other areas include whisker-or fiber-reinforced ceramic matrix composites that are being studied for a variety of high-temperature applications; ionic conductors for batteries, fuel cells, sensors, and gas-to-liquid fuel conversions; and advanced refractories for iron and steel making and for the containment of nuclear waste. Cements are being developed for some applications, rapid prototyping technology is also developed for the fabrication of ceramic parts. Generally, the Ceramics Section work includes microstructural characterization by optical and electron microscopy, phase identification by X-ray diffraction and differential thermal analysis, mechanical properties measurements, and for the superconductors, determination of critical current density and critical temperature. For composites, neutron diffraction is used to characterize the internal stress distribution. Those interested in hands-on ceramics laboratory work should apply for a position in this section.

729 MECHANICAL PROPERTIES OF METALS

Comp. Sci. Mat. Sci. Mech. Engr. Metal. Engr.

This section is involved in the study of mechanical behavior of structural alloys used in a number of energy systems. Group research activities include: (1) stress corrosion cracking, fatigue, and crack-growth behaviors of austenitic and ferritic steels in water-cooled nuclear reactor environments, (2) development and fabrication of advanced nuclear fuels, (3) testing and analysis of the structural integrity of nuclear reactor steam generator tubes, (4) computer analyses of structural components and tritium-breeding materials for fusion-reactor applications, and (5) failure analysis of actual components from nuclear power plants and other energy systems. Some projects involve laboratory testing of specimens under operating temperatures and pressures, while others rely on computer analyses to determine the expected materials behavior. This section offers the candidate the opportunity to work on real-world materials problems utilizing advanced mechanical testing equipment and environmental control systems, sophisticated microstructural characterization instrumentation, and advanced computer systems and software.

730 ANALYSIS AND MODELING OF MATERIALS BEHAVIOR IN ENERGY SYSTEMS.

Comp. Sci. Math. Mech. Engr. Metal. Engr. Nucl. Engr.

A modern, high-speed, digital computer is employed to simulate the physical behavior of materials used in advanced energy systems (fission and fusion). In the fission area, the thermal, mechanical, and irradiation response of fuel elements for the reduced enrichment research and test reactor (RERTR) is analyzed. Emphasis is placed on realistic models that accurately describe the physical situation. The DART code system is being developed in order to assess the behavior of dispersion fuels for the RERTR. In the fusion area, the thermal, mechanical, and irradiation performance of solid breeders (Li_2O and other ternary oxides) are being modeled. The TIARA code has been developed, verified and validated to predict the tritium inventory in lithium ceramics under fusion reactor operation conditions. Other research activities include the analysis of specific phenomena (e.g. helium-induced swelling) in order to identify key process and/or physical parameters that affect material performance. Finally, the response of plasma-facing components in fusion reactors to plasma disruption events is being analyzed.

731 COMPATIBILITY OF STRUCTURAL MATERIALS WITH LIQUID LITHIUM

Mat. Sci. Mech. Engr. Metal. Engr.

The program involves experimental studies to investigate the influence of chemical environments on the compatibility, corrosion, and mechanical properties of structural materials under conditions of interest in fusion reactors. Test environments include liquid lithium and helium. The scope of the program includes development of stable insulator coatings on structural materials to reduce magnetohydrodynamic (MHD) effects in liquid metal systems. The research requires some background in the areas of mechanical testing, thermodynamics, electron microscopy, and X-ray diffraction techniques to evaluate the environmental effects.

732 IRRADIATION PERFORMANCE OF REACTOR MATERIALS

Metal. Engr. Metal. Engr. Nucl. Engr. Ceram.

The principal objective of the programs in the Irradiation Performance Section is to determine and assess the behavior of materials, principally fuels and claddings, in the environment of nuclear reactors. This environment results in neutron damage and chemical, metallurgical, and mechanical processes that occur over a wide range of elevated temperatures. The programs fall into two categories: (1) fuel system development for a number of reactor types, and (2) postirradiation characterization of materials from existing reactors. The fuel development activities include planning of experiments for irradiation in a reactor, the postirradiation examination of these experiments, postirradiation testing of materials and components, and the evaluation and analysis of the results. Programs in postirradiation characterization involve examinations, testing, and data analysis. The Section operates the Alpha-Gamma Hot Cell Facility (AGHCF), in which fuel elements are examined, and the Irradiated Materials Laboratory (IML), a smaller hot-cell in which the mechanical property testing is performed. Available research tools include optical metallography, SEM, electron microprobe analysis, and scanning Auger microscopy. Cooperative research programs are welcomed.

733 OXIDATION-SULFIDATION BEHAVIOR OF MATERIALS

Mat. Sci. Metal. Engr.

The program involves experimental studies to establish the mechanism of oxidation-sulfidation of model metallic and ceramic materials exposed to complex and multicomponent gas environments. The research will require background in the areas of thermodynamics and kinetics of gas-solid reactions and use of optical and electron microscopy techniques to elucidate the corrosion mechanisms.

734 CORROSION OF MATERIALS IN THE PRESENCE OF DEPOSITS

Mat. Sci. Mech. Engr.

The program involves experimental studies to establish the mechanisms of corrosion of heat-exchanger and gas-turbine materials in the presence of deposits that are generated during the combustion of coal and coal-derived fuels. The research will require background in the areas of thermodynamics and kinetics of gas-solid reactions and fluid-flow characteristics that influence the type and rate of deposit(s). A background in X-ray diffraction is desirable.

735 STRESS-CORROSION CRACKING OF LIGHT-WATER REACTOR MATERIALS IN SIMULATED COOLANT ENVIRONMENTS

Chem. Mat. Sci. Metal. Engr.

The program involves an experimental investigation of the influence of simulated reactor-coolant environments, under normal and off-normal water chemistry conditions, on the susceptibility of piping and structural materials to stress-corrosion cracking. The effect of microstructure of the materials, water chemistry (viz. oxygen, hydrogen and impurity concentrations, pH), and temperature on the rate and mode of crack growth is being determined for a range of loading conditions. Background in the areas of electrochemistry, electron microscopy, aqueous corrosion, and physical metallurgy are applicable.

736 ALLOY MODIFICATION FOR IMPROVED CORROSION RESISTANCE

Mat. Sci. Metal. Engr.

The program involves experimental studies to establish the composition and microstructure of surface layers (created by ion implantation, surface coating, laser annealing, etc.) that impart improved corrosion resistance in oxygen and oxygen-sulfur-chloride environments. A background in transmission electron microscopy and Auger Electron Spectroscopy is desirable.

Surf. Sci.

737 TRIBOLOGY

Comp. Sci. Mat. Sci. Metal. Metal. Engr. Phy. Surf. Sci. Tribo. Sci. & Engr.

This section is concerned with the development of materials and surfaces with low coefficients of friction and high wear resistance, especially for applications involving high temperatures and aggressive chemical atmospheres (e.g., low-heat-rejection engines). The research activities are divided into three areas: (1) characterization and analysis of surfaces and coatings, (2) modification of surface tribological properties by the implantation of ions and the deposition of coatings, and (3) friction and wear testing and analysis. The characterization methods include scanning and transmission electron microscopy, scanning Auger microscopy, optical microscopy, X-ray analysis and Rutherford backscattering analysis. Surface morphology, composition, purity, microstructure, crystal structure, and the distribution of implanted ions are determined. Ions are implanted into the surfaces of metals and ceramics to reduce the coefficient of friction and to increase the wear resistance of the surface, or to prepare the surface for the deposition of highly-adherent, low-friction, low-wear coatings. Ion-beam-assisted deposition (simultaneous coating deposition and ion-beam bombardment) as a means to develop highly-adherent, low-friction and low-wear surfaces is a major activity. A vacuum chamber containing dual electron-beam evaporation sources and ion implanters has been developed and is being utilized in this research. Thermal properties are also a major consideration since these materials are intended primarily for high-temperature applications. A friction and wear testing and analysis laboratory has been set up. A Tally-Surf surface-topology measuring system, high- and low-frequency oscillatory and unidirectional friction and wear testers for operation under low and high temperature and controlled-atmosphere conditions, and a microwave diamond-film deposition system are routinely used.

738 ELECTROMECHANICS AND SUPERCONDUCTIVITY APPLICATIONS SECTION

Elec. Engr. Mech. Engr. Phy.

Research in this area involves the design, development, and analysis of macro-scale devices, such as motors, energy storage coils, power transmission lines, fault-current limiters, bearings, levitated vehicles, etc., using high-temperature superconductors. The group also investigates high-efficiency conventional electric motors, active magnetic bearings, the use of pulsed magnets in aluminum forming, and the use of ac magnets to contain and stir liquid metals. Fabrication and experimental testing of prototypes are conducted in most instances. Major past projects have included the development of superconducting current leads that require an order of magnitude less refrigeration than conventional leads, and a superconducting bearing that holds the world's record for the lowest coefficient of friction. Present projects include the use of superconducting bearings in flywheel energy-storage systems with a goal of 90% efficiency on a diurnal basis. One of our previous students won second prize in the national Apparatus Competition of the American Association of Physics Teachers for a superconducting motor that he built while working in our group.

ENVIRONMENT, SAFETY AND HEALTH DIVISION (ESH)

The Environment, Safety and Health Division is responsible for providing technical support to ensure a safe work environment for Argonne employees. ESH division personnel are engaged in the wide scope of activities required to make recommendations for, and maintain safe work practices and conditions throughout the Laboratory. Activities include safety engineering, health physics services, industrial hygiene services, personnel monitoring, internal dosimetry, emergency management, training, fire protection, and safety analyses.

739 INDUSTRIAL HYGIENE

Bio. Chem. Envr. Sci. Indus. Hyg. Phy.

Industrial Hygiene provides sitewide guidance and technical support for control of workplace exposures to chemicals and physical agents, excluding ionizing radiation. Exposures to solvents, gases, vapors, dusts, and mists are measured using a variety of direct-reading instruments and personal sampling devices. Laboratory analyses are performed on workplace, environmental, and biological samples. Other activities involve exposure surveys for noise, ultraviolet light and microwaves, selection, fit testing and user training of respiratory protective devices, and particle collection efficiency measurements of high-performance air-cleaning systems. Projects are available concentrating on a specific aspect of occupational health. A wide variety of instrumentation is used, including infrared, electrochemical cell and photoionization type gas and vapor monitors, aerosol photometers, data loggers, noise and microwave meters, and laser-based fibrous aerosol monitors. Optical microscopy is used for particle and fiber analyses.

740 ANALYTICAL SERVICES

Chem. Comp. Sci. Envr. Sci. Health Phy. Phy.

This section is responsible for the radiochemical and chemical analysis of environmental, workplace, and bioassay samples to verify the effectiveness of the Laboratory's protection and control systems, and to obtain data required to demonstrate the Laboratory's compliance with environmental and safety regulations. Participants may gain valuable experience by participating in an on-going analytical laboratory function, as well as by pursuing a specific research project designed to improve the effectiveness of this section's operations. Research projects include development of analytical methods for radioactive, organic or inorganic environmental pollutants, improvement of calibration methods for radiation detectors and dosimeters, application of body radioactivity measurements in vivo, and development of computerized data storage and retrieval systems. Major equipment items include state-of-the-art radiation spectrometry systems; GC/MS, LC, and AA chemical analysis instruments; and a MicroVax II supermicrocomputer.

741 ERGONOMICS

Investigations and actions to prevent repetitine strain injuries and other workplace ergonomics hazards.

742 HEALTH PHYSICS

Chem. Envr. Sci. Nucl. Engr. Phy. Radio. Phy.

This group is involved in all phases of the radiation monitoring, hazard evaluation, exposure control, and experiment review activities connected with ANL programs that use radioactive materials and radiation producing devices. In addition, it provides radiological characterization and assessment studies for decontamination and decommissioning efforts. Specific areas of research and/or development activity that are presently of interest, include the following: stray neutron energy spectrometer studies around ANL accelerator facilities; analysis of various Bonner sphere unfolding codes for neutron energy spectra; development of monitoring techniques for transuranic elements; determination of the sensitivity of stack-effluent monitoring equipment for detection and measurement of hot-cell effluents; development of Health Physics training courses; qualitative and quantitative studies of the activation of accelerator components by intense particle fluxes; evaluation of field techniques for radiological characterization of soils and other contaminated materials; acquisition of improved field-spectrometry techniques; development of state-of-the-art microprocessor-based survey instruments; and evaluations of the management of Health Physics records. A wide variety of radiation instrumentation is available including state-of-the-art survey and laboratory instrumentation. The latest in hyperpure germanium spectrometry systems as well as an anticoincident annulus NaI system constitute but a part of the instrumentation inventory. Mobile laboratories are available for field measurements and emergency response capabilities. A wide variety of applied health physics and development experiences are possible.

743 INDUSTRIAL AND CONSTRUCTION SAFETY

Safety Engr.

This section is responsible for developing and supporting the implementation of the industrial safety and construction safety programs at the Laboratory. The goal is to protect employees from injury and public property from the losses caused by accidents.

Facility Inspec.

In the industrial safety area, you will be involved in inspecting facilities with an eye toward ensuring that standards are complied with.

Machine Guard.

Machines are looked at to ensure guarding is in place and that operations are conducted in a safe manner. This requires reviewing procedures and observing operations.

Elec. Safety

Electrical safety efforts concentrate in lockout/tagout, maintenance procedures and the interpretation and application of codes and regulations.

Accident Invest. & Report.

Accidents are investigated and statistics maintained to assist in accident prevention efforts and trending. Knowledge of *Harvard Graphics* and *Word Perfect for Windows* is desirable

Constr. Safety

Argonne Safety Exper.

The construction safety program offers an opportunity to learn first hand the complexities of construction activities. Along the way you will review for comments, contracts, safety programs, and job specific hazard analyses. You will have dealings with independent contractors and construction workers during briefings at pre-bid and pre-construction meetings and during field observations of activities. You will also gain experience in conducting thorough tool and construction machinery inspections.

We have available a hands-on operational safety engineering experience touching on a variety of interesting and exciting subjects.

744 ESH TRAINING

This section designs, develops, and presents training on environment, safety, and health (ESH) issues throughout the Laboratory. Training classes, courses, and programs response to various DOE, EPA, OSHA, federal, and state regulations, as well as identified environment, safety, and health training needs. Design, development, and implementation of training may involve work lab-wide with subject matter experts and with ESH Division professionals from varied ESH disciplines, including Industrial Hygiene, Environmental Protection, Health Physics, Safety Engineering, Fire Protection Engineering, and Emergency Management. Varied training needs provide multiple opportunities to undertake creative approaches to instructional design and performance technology. Curriculum design, course design, and the associated front end work that incorporates needs analysis, determination of entry characteristics and behaviors, development of performance objectives, and creation of instructionally sound testing mechanisms are used. Evaluation of training programs, courses, means of instruction, and instructor competence are facets of ESH Training. As a research and development facility, Argonne provides a setting that encourages innovative training approaches including the design, development, testing for efficacy, and application of such methods as Computer Based Training (CBT) and Web-based training (WBT).

ENVIRONMENTAL ASSESSMENT DIVISION (EAD)

The Environmental Assessment Division has developed a broad program of interdisciplinary, applied research and development, undertaken from a system's perspective. The staff addresses a wide range of issues associated with energy technologies, energy and environmental policy, and environmental and societal effects of resource and industrial development. Environmental and resource assessments are conducted by professionals with expertise in the hydrogeological, physical, social, and ecological sciences and in radiological and health risk assessment. Our policy staff consists of environmental lawyers, sociologists, land-use planners, and archaeologists, and provides sophisticated analyses of government policy and strategy options. Special areas of interest include pathway analysis and risk assessments including ecological and human health, technology assessments, environmental restoration, and spatial analysis. We are experienced in building multidisciplinary technical teams for specific environmental projects, since many of our programs require integration of a wide range of skills.

745 ATMOSPHERIC SCIENCES

Air Qual.
Comp. Model.
Envr. Engr.

Construction and operation of energy technology systems and other industrial activities are evaluated to assess their potential impacts on ambient air quality, climate, meteorology, and acoustic environment. The effectiveness of control technologies and related government regulations in mitigating these impacts is also evaluated. Air-quality databases and new and improved methods of modeling air pollutant emissions, environmental transport and transformation processes, and noise propagation are developed as part of this work. Models are developed and performance evaluations are conducted to address emerging health and safety issues and to give environmental managers additional information on uncertainty in model predictions for consideration in formulating national and international energy and environmental policies. In addition, hazard analyses and risk and consequence assessments are performed to determine the impacts from possible releases of nuclear, chemical and biological agents. Recent projects have provided guidance to government agencies in hazard analysis, risk management, emergency response, and pollution prevention.

746 ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT

Comp. Sci.
Civil Engr.
Envr. Chem.
Envr. Engr.
Geol.

The Division also conducts environmental compliance and remediation studies as part of a hazardous-waste assessment program for federal facilities. The work includes analyzing present and past waste-management practices at different sites with regard to possible contamination of air, soil, surface water, and groundwater. Regulatory impacts on waste management and environmental remediation are also analyzed. Restoration studies include preliminary assessments, remedial investigation, feasibility studies, risk assessment, hydrogeologic studies and modeling, and the development of sampling and remedial design strategies. Pollution prevention studies emphasize changes in production and processing, material substitution, improved waste management practices, and cost.

747 ENVIRONMENTAL COMPLIANCE ACTIVITIES FOR REMEDIAL ACTIONS AT DEPARTMENT OF ENERGY SITES

Ecol.
Econ.
Envr. Engr.
Envr. Sci.

The Division is responsible for providing oversight review, technical and regulatory consultation, and recommendations to DOE for the planning and execution of environmental restoration activities at certain DOE facilities under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) and Resource Conservation and Recovery Act (RCRA). Activities include the evaluation and documentation of potential health risks to workers and members of the general public from exposures to radioactive and chemically hazardous substances present at these sites and the assessment of alternative remedial action approaches.

Health Phy. *Geol.* *Nucl. Engr.* *Soc.*

748 HYDROGEOLOGY

Comp. Sci.
Geol.
Hydrol.
Math.

Analytical and numerical models of surface flow, groundwater flow and solute transport are developed and used to evaluate environmental contamination problems. Impacts to human health, endangered species, and the environment are quantified. Geostatistics, advanced scientific visualization, graphical database, multi-media, and virtual reality techniques are used to prepare, analyze, and communicate the results of these studies. This area is multi-disciplinary involving a wide range of skills and knowledge. The interaction of water, geologic materials, and contaminants is a general part of most environmental issues.

Envr. Engr. *Civil Engr.* *Envr. Sci.*

749 NUCLEAR MATERIAL TRANSPORT

Health Phy.
Math.
Nucl. Engr.
Phy.

This activity involves the assessment of radiological impacts resulting from the releases of radioactive materials from transportation of radioactive nuclear waste materials. The assessment requires the modeling of the transport of radioactive materials via various environmental pathways that would eventually lead to radiation exposure to humans. Modeling includes computer simulation of radiation transport, atmospheric dispersion, radionuclide pathways, and radiation health effects.

750 ENVIRONMENTAL SYSTEMS PLANNING AND COMPLIANCE

Engr.
Envr.
Engr.
Phy.
Sci.

Multi-media and medium-specific approaches are employed to assess and solve existing environmental problems at federal facilities. Specific activities include both analytical studies and field work such as development of planning and guidance materials; audits of environmental compliance at federal facilities and associated corrective action plans; presentation of workshops on environmental laws, regulations, and compliance; preparation of baseline surveys and emission inventories; development of database management and expert computer systems for environmental information and permits; and preparation of NEPA documents and management of the NEPA process for specific projects. DOE assistance also includes mitigation action-plan preparation to document requirements set forth in the NEPA document.

751 COMPUTER MODELING AND RISK ASSESSMENT

Health
Phy.
Math.
Comp.
Sci.
Nucl.
Engr.

Environmental risk assessment usually uses computer models to simulate the transport of contaminants (radionuclides and hazardous material) in the environment. A suite of computer models (the RESRAD family of codes) have been developed by the Division. These models simulate the transport of contaminants in all potential pathways and calculate the concentrations in various media. Risks are calculated as both radiological and chemical doses and morbidity and mortality risks. Model uncertainty is estimated using Latin hypercube/Monte Carlo technique. The RESRAD codes have been used to derive cleanup criteria for over 300 sites and it has been used as a teaching tool by many universities. These models are constantly being updated when new data/techniques are developed.

Phy.

752 ECOLOGICAL AND GEOGRAPHICAL SCIENCES

Ecol.
Envr.
Sci.
Bio.
Stat.
Model.

Analyses are conducted on the effects of human activities on aquatic, terrestrial, and wetland ecosystems, ecological communities, plant and animal populations, threatened and endangered species, and cultural resources. Impacts examined include hydrologic alteration, habitat effects, land disturbance, radiological and chemical contamination, and cumulative impacts. Ecological risk assessments are performed for contaminated sites to develop cleanup criteria and evaluate remediation alternatives. Mitigation or management strategies such as ecological restoration are developed to reduce impacts and enhance ecosystem function. Information is gathered through field and laboratory studies, remote sensing, and literature searches, and is analyzed using statistical techniques, modeling, and geographic information systems. Recent projects have examined the effects of dam operations on aquatic and terrestrial ecosystems in the Colorado River Basin biodiversity issues at Air Force stations habitat evaluations at Army installations and ecological risk assessments at Army disposal sites.

753 ENVIRONMENTAL POLICY ANALYSIS (Washington, DC location)

Envr. Engr. Health Sci. Soc. Eco.

Environmental, technology and economic implications associated with development and implementation of environmental policy, legislation and regulations are assessed. Multidisciplinary and focused assessments are conducted within a wide scope of environmental topics. Results of assessments including pollutants emissions and environmental impact projections, environmental control and remediation costs, guidance and training courses and materials, and options analysis provide input to environmental policy decision-making.

Law Envr. Sci.

754 NATURAL RESOURCES

Ecol. Hydro. Nat. Resources Forestry Fish & Wildlife

Natural resource management plans are prepared for federal facilities that identify goals and objectives for a five-year period. An integrated approach is taken to develop the plans that examines planned facility missions and programs, potential impacts associated with each program, and current baseline physical and natural environment. Program activities are considered together with objectives for fish and wildlife management, forestry resources, federal and state protected species, recreational programs, wetland resources, waste management and cleanup, and adjacent land use. Integrated natural resource management plans are then used to develop detailed operational plans that describe specific tasks, associated labor effort, cost, and final products anticipated by implementing the tasks to meet overall plan objectives.

755 ENVIRONMENTAL IMPACT ASSESSMENT

Nat. Sci. Pol. Sci. Soc. Sci.

Proposed federal actions are assessed according to the requirements of the National Environmental Policy Act (NEPA). Environmental effects are analyzed and presented in environmental impact statements and other documents. Activities include conducting public involvement activities, gathering information and data, evaluating environmental impacts, development of databases and multi-media tools, response to issues of public concern, examination of regulatory issues, information retrieval and archiving, development of management tools, and report preparation. These activities are performed by closely integrated multi-disciplinary teams.

756 RISK ASSESSMENT

Health Phy. Health Sci. Ecol. Envr. Model.

Risk assessment is used as a tool in determining environmental management objectives and in evaluating a wide range of technological and environmental issues in various land-use and demographic settings. In conducting these assessments, an extensive set of analytical tools are used to quantify the hazards or sources of risk, the pathways or mechanisms by which sensitive human or ecosystem populations become exposed, and the nature and extent of the resulting impacts. One such tool is the RESRAD computer code which determines site-specific cleanup guidelines on the basis of the calculated exposures to hypothetical residents or workers on the site. Other focus areas include evaluations of transportation risks, risks to the ecosystem, probabilistic risk assessments, and risk communications.

Envr. Sci.

ENVIRONMENTAL RESEARCH DIVISION (ER)

Research activities in this division include a broad spectrum of fundamental and applied investigations into the functioning of the environmental systems, particularly in response to anthropogenic stresses. Consequently, the information derived from the various research projects addresses critical environmental issues that face society. Current emphasis is on the environmental effects of hazardous wastes (e.g., identification, amelioration, and remediation) and atmospheric responses to energy production and use (e.g., induction of acidic rain and alteration of global climate). The Division is organized into two scientific sections (Atmospheric Research and Terrestrial Research), each with several research groups, as well as three major additional program groupings (Environmental Management and Surveys, Photophysics and Photochemistry, and Radiation Physics). An interactive and collaborative approach to the investigation of these complex environmental issues is the hallmark of the Division.

ATMOSPHERIC SECTION

Research activities include investigation of the physics and chemistry of the lower atmosphere, particularly with regard to the processes of transport, chemical transformation, diffusion, and deposition of airborne trace substances. Related activities involve studies of climate change and aquatic environments in freshwater lakes. Factors that influence the behavior of pollutants are measured with a view toward the development of descriptive theoretical and numerical models. Particular attention is paid to the changes in the atmosphere that are brought about by human activities, such as emissions from the burning of fossil fuels.

757 ATMOSPHERIC PHYSICS

Chem.
Elec.
Engr.
Meteor.
Phy.

Field studies and modeling are emphasized. GLOBAL CHANGE studies use observational facilities in the Southern Great Plains to study processes that are important in climate modeling. Improved subgrid-scale parameterizations are developed for the structure of the planetary boundary layer and the air-surface exchange of heat, moisture, and solar and infrared radiation. REMOTE SENSING from the ground uses Doppler acoustic, radar, and laser systems along with *in situ* observational systems to study the structure of the planetary boundary layer and to evaluate the transport and dispersive properties of the lower atmosphere above complete terrain. Satellite data on optical radiance reflectances from land surfaces are used to study energy balances and the corresponding biological properties that affect energy flows. The heat, water vapor, and carbon dioxide fluxes are evaluated over large areas with models and results are compared to local observations made in the field. NUMERICAL MODELS are developed and applied to study the structure of planetary boundary layer as it affects energy flows, meteorological conditions, and the transport and dispersion of trace chemicals.

758 ATMOSPHERIC CHEMISTRY

Chem.
Elec.
Engr.
Meteor.
Phy.

The chemistry and fates of energy-related trace chemicals in the atmosphere are studied over continental areas. The research concentrates on the behavior of ozone, nitrogen, and sulfur gases; volatile organic compounds; organic oxidants; and fine particles. The turbulent air-surface exchange of the substances is measured in dedicated field experiments, parameterizations of the exchange rates are developed, and models are developed to use satellite data to describe the exchange rates over regional and global scales. Observations of organic compounds are taken at the surface and aboard research aircraft during field experiments, and the data are used to evaluate the processes that generate ozone and other oxidants in the atmosphere. Laboratory and field studies of organic oxidants are carried out because they are key secondary pollutants that play important roles in the gas, aerosol, and aqueous phase chemistry in the troposphere and can be toxic to plants and animals. In addition, many of the substances affect climatologically important radiative transfer processes by acting as greenhouse gases or by contributing in particulate form to the scattering and absorption of radiation. Many of the findings from the observational studies are interpreted and generalized with the use of numerical models of atmospheric chemistry and transport.

759 AQUATIC PROCESSES

Appl.
Comp.
Envr.
Sci.

A variety of techniques are used to study both climatic effects and contaminant transport and exchange processes in the Great Lakes and the Great Lake region. These include analysis of data obtained from satellites, collection of ***in situ*** observations of the benthic boundary layer, numerical modeling, and statistical analysis of water-quality data. Advanced procedures such as optimization and inverse analysis are used as well.

Phy.

TERRESTRIAL SECTION

Research activities conducted in this area involve both field and laboratory investigations on the transport, fate, and biogeochemical behavior of hazardous wastes, including radionuclides. Other studies address the effects of environmental stresses on terrestrial ecosystems, both natural and managed. Environmental stresses include such things as air pollutants, acidic rain, and ozone. Disturbance effects studies examine changes to ecosystems resulting from stresses associated with energy production and use.

760 MICROBIOLOGY

Bio.
Bio-Chem.
Bio-tech.
Micro-bio.
Molec. Bio.

Microbes can convert cheap, renewable resources to valuable products and have long been exploited for this ability. Efforts are now in progress to expand their use to include the production of larger-volume, less-expensive chemicals. New processes and products to be developed will reduce both dependency on petroleum and the environmental liabilities of some industrial chemicals. At Argonne, modern techniques in microbiology, genetic engineering, and enzymology, as well as classical approaches, are being applied in this effort. Addition of foreign genes or alteration of gene expression, called "metabolic engineering", attempts to alter the metabolic pathways of the microbes to produce different chemicals. Site-specific mutagenesis of proteins attempts to change the specificity or stability of enzymes to create novel catalysts that will carry out useful reactions not performed by naturally occurring enzymes. Strains developed by these approaches are evaluated in laboratory scale fermentations, which are then optimized for production of the desired metabolites.

761 TERRESTRIAL ECOLOGY

Bot.
Ecol.
Envr.
Sci.
Field.
Bio.

The significance of symbiotic mycorrhizal fungi in the long-term survival of host plants has not been well-documented. Research is being conducted on the influence of mycorrhizal fungi on host and nonhost plant survival as it relates to ecosystem recovery, especially as to how this association affects the fitness of the host, both directly and indirectly. In other studies, plant-soil interactions are investigated from the standpoint of the plant-soil interface in a range of systems from row crops to native tallgrass prairie. Field and laboratory studies are conducted to determine the interrelationships between plant roots, associated symbiotic microflora, developing soil structure, and ion and water availability.

Microbio.

762 ENVIRONMENTAL GEOCHEMISTRY

To understand and predict the behavior of contaminants in subsurface environments requires additional fundamental research. n the Geochemical Processes Group, we are pursuing two major areas of research in environmental geochemistry. One is the application of synchrotron x-ray scattering and spectroscopy methods to in-situ studies of mineral-fluid interfaces. This work is performed at the Advanced Photon Source. We are developing state-of-the-art methods for investigation of the molecular-scale structures and reaction mechanisms that control the behavior of metal and organic species in soils and groundwaters.

The other area of research involves the application of precise stable isotope measurements for investigating the biodegradation of chlorinated aliphatic hydrocarbons (CAHs). In this work we perform laboratory experiments to measure biological isotope effects during degradation of CAHs, and we also collect groundwater samples from contaminated fields sites. The isotope ratios of carbon and chlorine are measured for residual CAHs and their degradation products (e.g., chloride and bicarbonate). From these isotopic measurements, it is possible to determine whether biodegradation is occurring, and if so, to estimate the extent of CAH biodegradation in the groundwater aquifer.

763 SYNCHROTRON-BASED ENVIRONMENTAL RESEARCH

This research program in synchrotron-based environmental research is aimed at exploring applications of new advances in x-ray physics to understanding problems in environmental science. The principal goal of this program is to address general issues concerning the bioavailability of contaminants in the environment, with a particular emphasis on the mobility, uptake mechanisms, transformations, and toxicity of metals and organic chemicals in natural soils. Research projects include both the study of bulk samples by using x-ray absorption spectroscopy and the study of microscopic samples and spatial variations on the micron length scale by using x-ray fluorescence imaging, phase contrast imaging, and x-ray absorption spectroscopy with micron-sized spots.

764 APPLIED GEOSCIENCE AND ENVIRONMENTAL MANAGEMENT AND FIELD RESEARCH

Comp. Sci.

Envr. Asses.

Field Bio.

Argonne's program in applied geoscience and environmental management is exploring the adaptation of nonintrusive geophysical and geochemical techniques used in petroleum exploration and mining to produce data sets that can, for example, be integrated with geology to identify contamination and predict directions of contaminant migration in field sites. Nonintrusive techniques being adapted include seismic refraction and electromagnetic surveys, geochemical analyses and analysis of stable isotope tracers. The integrated results are used to prioritize potential sampling locations on the basis of their potential usefulness in pinpointing contaminants, thus limiting the need for costly drilling and analytical work. This process is called Argonne Expedited Site Characterization (ANL/ESC). The ESC process has been used in remedial site characterization programs for numerous hazardous waste sites. The first step in the process is to generate sound geological and site history models that guide the selection of appropriate geological, geochemical, and geophysical techniques. An integrated team of scientists then goes to the field and collects the variety of results that are then combined to determine the extent of the contamination. The process is quick and cost-effective. The significant results of the integrated ANL/ESC approach include: (1) identification of principal controls on subsurface migration pathways of contaminants, (2) improved geochemical sampling programs, (3) better delineation and prediction of the nature of the aquifer system, including confinement, water table levels, and geologic controls, (4) identification of relevant subsurface features (old trenches, geologic faults, or aquitards, for example) that are often missed with more traditional approaches, and (5) a reduced number of required wells for long-term monitoring of the site.

HIGH ENERGY PHYSICS DIVISION (HEP)

This Division conducts research into the nature and properties of elementary particles--the building blocks of matter. The program includes colliding beam experiments at the proton-antiproton collider (TeV-1) at nearby Fermi National Accelerator Laboratory. The structure of the proton is being studied at the HERA electron-proton collider in Hamburg, Germany. The effects of spin in elementary particle scattering are being studied over a wide range of energies. Research not requiring particle accelerators includes construction of a major underground detector to search for proton decay and the use of superspeed multinode processors for lattice gauge computations. The Division's theoretical group is active in several areas of elementary particle theory. Accelerator physics research includes development of new acceleration techniques and designs for new accelerator facilities.

765 LEPTON SCATTERING EXPERIMENTS

Engr.

Phy.

Physicists from Argonne's High Energy Physics Division, together with colleagues from 50 institutions from different parts of the world, are involved in studies of high energy electron-proton collisions. The experiment ZEUS, is located at the HERA colliding beam facility at the DESY Laboratory in Hamburg, Germany. With energies of 27 GeV for the electrons and 920 GeV for the protons, the structure of the proton is being probed with unprecedented accuracy. A large variety of physics topics are being addressed: structure functions of the proton, photon, and pion, diffractive scattering, searches for exotic particles, etc.

A group of U.S. institutions was responsible for the design and construction of the barrel calorimeter, one of the major components of the experiment. In an effort to improve the performance of the ZEUS detector, the Argonne group built a preshower counter that will is located in front of the barrel calorimeter. There are opportunities for students as well as faculty to become involved in both the data analysis and the hardware upgrade.

766 MINOS LONG BASELINE NEUTRINO EXPERIMENT

Engr.

Phy.

Cosmic ray experiments suggest that the phenomenon of neutrino oscillations have been observed. This implies that a neutrino which is produced in one of the three flavors might interact as a different flavor neutrino. In particular, it is believed that muon neutrinos are oscillation into tau neutrinos. This implies that neutrinos have a small but finite mass.

A large group of physicists from Argonne and around the world are building a 5000-ton neutrino detector in the Soudan mine in Minnesota to use in conjunction with a new neutrino beam from Fermilab. A smaller version of the "MINOS" neutrino detector will be built at Fermilab. There are opportunities for students and faculty to be involved in the simulation and analysis of data for the new experiment, and for work on electronics and scintillator components for the new detector.

767 EXPERIMENTS USING POLARIZED BEAMS

Phy. This program consists of two experiments, one studying the spin dependence of proton-proton interactions at high energies, and the other kaon-proton interactions producing lambda and sigma hyperons at the intermediate energies. Both of these experiments are international collaborations involving many physicists.

The Argonne group is involved in the Relativistic Heavy Ion Collider (RHIC) spin experiments at Brookhaven National Laboratory. Detailed tasks include design and construction of a polarimeter for RHIC and an endcap electromagnetic calorimeter for one of the large RHIC detectors (STAR). The primary physics issues that will be studied at center of mass collision energies from 100 to 500 GeV are: (1) the spin content of the proton, including measurements of the gluon and sea quark helicity distributions; (2) checking of the electroweak couplings including parity violation in $W^{\pm}$ and Z° production; and (3) measurements with transversely polarized beams. To achieve these physics goals, there will be detection of jets, direct photons, $W^{\pm}$'s, and Z°'s; the endcap calorimeter will play a crucial role in these measurements.

The group is also participating in studies of kaon-proton interactions at Brookhaven using the SLAC Crystal Ball detector. This detector consists of 672 Nal detectors covering almost 4π solid angle for measurement of photon and neutron land sigma resonant states. Some decay channels allow the determination of spin asymmetries due to the weak decays of hyperons. Many challenging pattern recognition problems are being studied.

768 PROTON-ANTIPROTON COLLIDER EXPERIMENTS

Phy. This activity is part of an international collaborative effort to study proton-antiproton collisions using the Collider Detector at Fermilab. The 1800.GeV center-of-mass collision energy is the highest currently available in particle physics, and has opened up new possibilities for studying phenomena. The detector contains a large solenoidal magnet with extensive charged-particle tracking devices, including silicon microvertex detectors completely surrounded by calorimeters. The central electromagnetic calorimeter design and construction was led by the Argonne group. More than 100 pb^{-1} of integrated luminosity has been obtained running at the Tevatron Collider.

This sample continues to be used to make precision measurement of the W gauge boson mass, and following the discovery of the top quark determining its mass and studying production properties. Our group is also involved in studying the strong interaction and proton structure using direct photon production and aspects of b-quark.

The Collider Detector at Fermilab is now in an extensive upgrade program, preparing for the higher intensities which will come from accelerator upgrades, including the new Main Injector. The Argonne group is involved in new electronics for the electromagnetic calorimeter, the new central drift chamber, and other areas.

769 ACCELERATOR PHYSICS GROUP

Elec. Engr. Phy. Comp. Sci.

Experimental and theoretical studies are in progress to develop new and better techniques for particle acceleration. Such techniques will be required to permit future explorations of physics at the highest energies. Argonne pioneered a new experimental technique which uses a precisely time relativistic electron beam to probe high-gradient electric fields, "wake fields", which are produced by a leading high-current "drive" pulse. With it, new insights have been gained about wake fields in plasmas and in a wide variety of passive structures.

The first phase of a new facility is now operating which will extend experiments beyond "proof of principle" into technologically interesting levels. It includes a high current (up to 10 kA) laser photocathode based electron gun, a special rf linac to handle the large current, a separate low intensity gun which forms the "probe" beam, and a well-instrumented experiment section. With it, accelerating gradients of 100-300 MeV/m will be studied and demonstrated.

Many technical subjects are relevant to this project, including laser and particle beam physics, microwave properties of materials, magnet and cavity design, accelerator theory, and computer simulation.

770 ATLAS DETECTOR AT LHC

Comp. Sci. Elec. Engr. Phy.

Argonne physicists have joined the large collaboration planning to build the ATLAS detector at the LHC (Large Hadron Collider), the next accelerator to be built at CERN, the European Organization for Nuclear Physics. ATLAS will be a large general-purpose detector with several major subsystems: inner (tracking) detector, superconducting solenoid, electromagnetic calorimeter, hadronic calorimeter, and muon system. The high energies that will be available at LHC are expected to provide insight into several of the puzzles of current particle physics, including the origin of electroweak symmetry breaking and the hierarchy of particle masses. Argonne plans a major role in design and protyping of the hadronic calorimeter which is based on scintillating tile technology. These tasks are now essentially complete and construction proper commenced in January 1999 with the construction of the first sections (submodules) of the absorber structure. Construction of the submodules will continue for the remainder of 1999 and 2000. In addition, in the summer of 1999, we will commence construction of the first modules, which are assembled from the submodule section as well as its instrumentation and testing using light and/or radioactive sources. The first of these production modules will be tested at CERN with high energy particle beams.

Argonne physicists are also involved with detector triggering and with offline computing development. Ongoing activities include tests of prototype hardware, both as components and as elements of a partial trigger system as well as simulation of the triggers to be implemented.

For offline computing, the group is investigating new software architectures based on Object-Oriented methods and has written prototype sections of the software system. The prototype work will continue for the rest of 1999 and into 2000, at which point we hope to have developed a full implementation for use in analysis of data taken in the beam tests of the first production calorimeter modules.

INDUSTRIAL TECHNOLOGY DEVELOPMENT CENTER (ITD)

The Industrial Technology Development Center is the focus for transferring Argonne technology to industry and for cooperative programs with industry. The Center's activities include developing jointly funded research and development programs with industry, evaluating and licensing inventions, and arranging access to Argonne's research facilities by industrial organizations. Opportunities are available in ITD to:

771

- Evaluate Argonne inventions for value to industry, and to identify potential fields of application.
- Develop and perform follow-up surveys of the effectiveness of various ITD activities.
- Participate in MS-DOS personal-computer-based activities, including developing and improving databases and providing technical support to ITD staff relative to business application programs.

INTENSE PULSED NEUTRON SOURCE DIVISION (IPNS)

The Intense Pulsed Neutron Source Division (IPNS) operates an accelerator-based source of neutrons for basic research in condensed matter using neutron-scattering techniques. The IPNS program is operated in a user-oriented mode with thirteen neutron-scattering instruments. Research using these facilities is sponsored by various research divisions.

772 IPNS DATA ACQUISITION AND ANALYSIS

Bio.
Chem.
Comp. Sci.
Elec. Engr.
Mat. Sci.
Phy.

IPNS uses computers to collect and analyze neutron scattering data. The data collection process involves recording the time-of-flight of detected neutrons and binning the data in histograms. This is done through a dedicated microprocessor. We are in the process of converting the control of this system from a MicroVAX system to a Linux system. Old Fortran codes are being rewritten in C or Java. We are currently in the process of modernizing the data acquisition hardware and software. Older Multibus and CAMAC modules are being replaced with VSI/VME modules residing in crates that sit directly on the network and communicate with the outside world using EPICS (Experimental Physics and Industrial Control System). This allows more freedom in the choice of user interface computer and gives the possibility for user interfaces to be developed on a variety of platforms such as Unix, Windows, VMS, etc.

We are also in the process of developing a network-based data display and visualization program. The software is being written in the Java language so it will run on any modern computer platform without being recompiled or rebuilt. This will also allow running the software through a web browser.

Research participants would assist in the development of code for experiment control or for data collection, with emphasis on conversion of codes to Unix. They might also assist in writing object-oriented codes in Java for setting up data collection or manipulating and displaying data. The students will learn or gain experience in object-oriented programming techniques.

773 IPNS ACCELERATOR SYSTEM

Comp. Sci.
Elec. Engr.
Mech. Engr.
Phy.

The IPNS accelerator system is an operating facility consisting of an H^- ion source, a 750-keV Cockcroft-Walton dc preaccelerator, a 50-MeV Alvarez linac, and a 450-MeV Rapid-Cycling Synchrotron. Computer science projects include work on EPICS[1]-based data acquisition and control systems, development of man-machine interfaces and graphical presentation of data. Particle accelerator technology features high-current regulated magnet power supplies; frequency, amplitude, and phase-modulated high-power rf transmitters; vacuum systems; analog and digital control with feedback circuits; and dedicated computer-control systems. Improvements and modifications to various systems and investigation of beam performance is continually ongoing, providing the participants with a unique experience in computer science, the physics of charged-particle dynamics, as well as a wide variety of engineering specialties.

[1] EPICS (Experimental Physics Instrumentation and Control Systems) is an Argonne/Los Alamos developed system that is now used at over 100 sites.

774 IPNS NEUTRON PHYSICS

Mat. Sci. Nucl. Engr. The IPNS neutron-generating system consists of a depleted uranium target having nearby liquid and solid methane moderators for slowing the neutrons down to energies appropriate for neutron-scattering studies. Participants will assist senior staff on a variety of measurements to characterize target, moderator, and instrument performance. Target/moderator programs include measurements of pulse shape, neutron spectra, energy deposition, radiation damage in the moderators, and measurement and analysis related to the management of thermochemical instability in solid methane; and energy deposition, delayed neutrons, and shielding of the uranium target. Instrument programs include the design, testing, and characterization of instrument components and systems for neutron detection, shielding and background reduction, and neutron optics in neutron-scattering instruments.

775 IPNS NEUTRON SCATTERING RESEARCH

Bio. Chem. Mat. Sci. Phy. The IPNS neutron scattering facility consists of 13 instruments for investigating the structural and dynamical properties of condensed matter. The neutron-scattering instruments include 7 diffractometers (for structures in powders, single crystals, glasses, liquids, and soft materials), 4 spectrometers (for magnetic and chemical excitations, atomic/molecular vibrations and diffusion with energy transfers from 0.05 to 1500 meV), and 2 reflectometers (for interfacial magnetic and atomic structure). Over 300 experiments are performed per year in various areas of materials sciences, physics, chemistry, biology, and applied technology. Recent studies include the structure of high-temperature superconductors, high-temperature properties of ceramics, interdiffusion of polymers, formation and structure of zeolites and catalysts, intermediate range order in glasses, residual stresses in composites, magnetic excitations in transition-metal compounds, and neutron irradiation studies.

MATERIALS SCIENCE DIVISION (MSD)

This Division conducts basic research on metals, alloys, ceramics -- including high-T_C superconductors -- and glasses that could have applications in advanced energy systems. The research programs are focused on the structure and properties of materials under extreme conditions of temperature, pressure, radiation flux, and chemical environment. The Division is a major user of the Intense Pulsed Neutron Source (IPNS) and synchrotrons, and operates the high-voltage electron-microscope Tandem-Accelerator System as a national user facility.

776 MAGNETIC FILMS

Chem.
Elec.
Engr.
Mat.
Sci.
Phy.

This group prepares and characterizes ultrathin films with novel properties. The materials are prepared as surfaces, interfaces, heterostructures, sandwiches, and superlattices using molecular-beam epitaxy and sputtering techniques. Interest focuses on magnetic, superconducting, optical, transport, structural and elastic properties of predominantly magnetic systems. Characterization techniques include ultrahigh-vacuum electron spectroscopies and diffraction, light scattering (Raman, and Brillouin), magneto-optic Kerr effect, magnetometry, magnetotransport and x-ray diffraction. Participants aid in film preparation, and analysis and modeling of physical properties. Data handling via computer is usually part of the assignment.

777 APPLIED SUPERCONDUCTIVITY

Chem.
Elec.
Engr.
Mat.
Sci.
Phy.

This research concentrates on high-temperature oxide superconductors. It addresses materials fabrication and fundamental scientific issues that affect the end uses of these materials. As an example, characterizations of these materials by transmission electron microscopy help to bridge the connection between current carrying capability and fabrication conditions so that better materials can be made. Thus an important properties characterization involves low temperature electrical conduction measurements (made down to a temperature of 2K) using superconducting magnets to provide fields of up to 9T. We study the magnetic flux lines which penetrate the superconductor in a field with aim of better understanding their dynamics. This is of great interest from the point of view of fundamental physics, but is also very important for high current applications since flux motion leads to voltages within the superconductor and thereby the loss of perfect conduction.

778 BASIC SUPERCONDUCTIVITY

Chem.
Elec.
Engr.
Mat.
Sci.
Phy.

Our research includes both experimental and theoretical investigations into the physics of a wide class of magnetic and superconducting materials. Current activities are concerned primarily with characterizing the electronic properties of high temperature ceramic superconductors and organic superconductors. Experimental techniques include de Haas van Alphen quantum-oscillation measurements at very-high magnetic fields and low temperatures, magneto-transport measurements, scanning tunneling microscopy, magnetization measurements with superconducting quantum interference devices (SQUID), and AC susceptibility studies up to 10 Tesla. In addition, we have recently fabricated a state of the art magneto-optics installation to visualize magnetic flux motion in real time. Participants will be involved with a variety of measuring techniques and instrumentation, and learn through hands-on experience the fundamentals of experimentation including computer interfaces.

779 NEUTRON AND X-RAY SCATTERING

Chem. *Elec.* *Engr.* *Mat.* *Sci.* *Phy.*

Members of the neutron and x-ray scattering group pursue multidisciplinary research programs of the nature that are only possible if scattering capabilities are combined with other experimental work. Major research programs include: high-T_c superconductors, colossal magnetoresistive materials, ceramic membrane reactor materials, negative thermal expansion materials, magnetic response of strongly correlated electron systems, a wide range of disordered materials including glasses, liquids, and polymer electrolytes, and multilayer and amorphous magnetic systems. A second important goal of the group is to provide the technical expertise required to continue the development of a future advanced pulsed neutron source. Scientists in the group play a lead role in the development of new instrumentation and user-based research programs at the Intense Pulsed Neutron Source (IPNS) and serve as instrument scientists for five instruments at the IPNS. Members of the group are becoming involved in the development of instrumentation for the Spallation Neutron Source at Oak Ridge National Laboratory and are also active in developing new x-ray scattering instrumentation and techniques for use at the Advanced Photon Source and other synchrotron x-ray sources.

780 SYNCHROTRON RADIATION STUDIES

Chem. *Elec.* *Engr.* *Mat.* *Sci.* *Phy.*

The synchrotron radiation studies group utilizes a variety of X-ray scattering techniques ranging from single-crystal and powder diffraction for structure determination, x-reflectivity and standing-waves for the study of surfaces; to X-ray absorption spectra (EXAFS and XANES), photoelectron spectromicroscopy, and angle-resolved UV photoemission measurements for the study of electronic structures of materials. These studies are carried out with in-house X-ray scattering instrumentation and at synchrotrons at Brookhaven (NSLS), Cornell (CHESS), Stoughton (SRC) and the Advanced Photon Source at Argonne, to provide information on the structural and electronic aspects of materials of interest to both group members and other researchers in the Materials Science Division. Of particular interest are chemical and electronic structures of high-temperature superconductors and the study of structures of surfaces and interfaces. Participants are invited to join with a group member in research of mutual interest or to contribute to on-going research efforts.

781 CONDENSED MATTER THEORY

Chem. *Elec.* *Engr.* *Mat.* *Sci.* *Phy.*

Projects are available in a variety of areas involving analytical and numerical simulations of simple models of the behavior of condensed matter. Past participant projects included studies of various properties of superconductors: microscopic and phenomenological theories, vortex lattices, high T_C, heavy fermions, etc.; electronic structure and properties of strongly correlated metals., magnetic multilayers, quantum effects in electronic kinetics, particularly, in strong magnetic fields. Participant responsibilities include analytical solution of simple problems, programming and running the simulations and participating in discussions of their scientific implications. Participants will have the opportunity to use supercomputers and parallel processors.

782 RADIATION AND KINETICS EFFECTS

Mat. Sci.
Metal. Engr.
Nucl. Engr.

Fundamental mechanisms that induce microstructural changes during irradiation are studied. Investigations of surface modifications by ion beams are directed toward understanding processes (such as ion beam mixing, radiation-enhanced interdiffusion, and sputtering) that produce surface layers with properties significantly different from those of bulk material. Research on radiation-induced segregation and defect production is providing a fundamental basis for the engineering of materials tailored to specific applications in both fission and fusion radiation environments. Additional studies focus on fundamental properties, defects, and irradiation effects in high-T_c superconductors.

Phy.

Emphasis is placed on experimental techniques that allow quantitative information about microstructural changes to be obtained in situ, e.g., ion beam analysis, Auger depth-profiling, and conventional and analytical electron microscopy. Computer and analytical modeling are used in support of the experimental activities.

783 CERAMIC EPITAXIAL FILMS AND COMPOSITES

Chem.
Elec. Engr.
Mat. Sci.
Phy.

Thin-film ceramic materials are widely used in a variety of device applications with significant economic impact. The physical properties of such films differ from bulk properties because of epitaxial strains and growth defects resulting from lattice mismatch and other interfacial effects. This program focuses on the processing, characterization, and property determination of single-crystal and polycrystalline epitaxial ceramic films and layered composites prepared by metal-organic chemical vapor deposition (MOCVD) techniques and by means of atomistic computer simulations (the latter involving lattice statics, lattice dynamics, molecular dynamics and Monte Carlo techniques). The main objectives are twofold, namely (a) to enhance our fundamental understanding of the processing-structure-property relationship of thin ceramic films and multilayers and (b) to measure and/or simulate tensor properties of single-crystalline films, thus elucidating the physical basis for the performance of these materials. In the past, devices using these materials have been made almost exclusively in polycrystalline form. Our main emphasis is on electro-ceramic materials, involving their dielectric, piezoelectric, electro-optic, acousto-optic and elastic behavior, with particular emphasis on the role of interfaces, such as grain and phase boundaries.

784 INTERFACES IN ADVANCED CERAMICS

Ceram.
Chem.
Mat. Sci.
Nucl. Engr.
Phy.

This program addresses interface (epitaxy, grain- or phase-boundary) related properties of advanced ceramics and ceramic composites, with particular emphasis on atomic-level investigations of the structure and chemistry of the interfaces in these materials. Advanced ceramic materials are used, for example, as electronic-packaging materials, in structural applications, in advanced batteries and fuel cells, as ceramic-coating materials or as high-T_C superconducting materials. In this program we are combining advanced methods for the synthesis of these materials in nanophase, multilayer and/or thin-film form with atomic-level experimental characterization techniques and atomistic simulations (the latter involving lattice statics, lattice dynamics, molecular dynamics and Monte Carlo techniques). This enables us to address fundamental issues of relevance to the processing and mechanical performance of advanced ceramics. Among these issues are, for example, (a) the relationship between microstructure, atomic structure and interface chemistry (incl. non-stoichiometry and interfacial phases) as a function of processing conditions, (b) the role of amorphous interface phases and (c) point-defect and mechanical properties. The program draws heavily on three major Argonne facilities, the Electron Microscopy Center (HREM, AEM) and, in the near future, the Advanced Photon Source, as well as Argonne's expertise in massively parallel computing architectures.

785 ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

Ceram.
Comp. Sci.
Elec. Engr.
Mat. Sci.
Metal. Engr.
Nucl. Engr.
Phy.

Research in the Electron Microscopy Center is directed toward the experimental determination of the morphology, crystallography, elemental and chemical composition, and electronic structure of phases, interfaces, surfaces, and defects present in pure elements, alloys, ceramics, and other technologically important materials. State-of-the-art transmission and scanning-transmission electron microscopes (TEM/STEM's) as well as a 1.2-MeV high-voltage electron microscope (HVEM) are employed to characterize the microstructure of solids using conventional diffraction contrast techniques. Quantitative analytical information is obtained through the use of X-ray energy dispersive and electron energy-loss spectrometers for elemental, chemical, and electronic structure studies interfaced to the above instruments. This analytical information is obtainable from regions that can be as small as 10 nanometers in diameter. Investigators can choose to concentrate on applications of transmission electron-microscopy-based techniques to characterize materials, or research on fundamental (experimental or theoretical) studies of electron/solid interactions to advance state-of-the-art understanding and techniques for characterization. When appropriate, joint appointments between the Electron Microscopy Center and various MSD research groups will be suggested.

786 LASERS IN SURFACE SCIENCE

Chem.
Metal. Sci.
Metal. Engr.
Phy.

An extremely sensitive method of examining the chemical composition of a surface is to ionize and detect neutral atoms and molecules ejected from a sample during ion-, electron-, or photo-stimulated desorption. For most surfaces >99.9% of the desorbed atoms and molecules are charge neutral, and therefore undetectable in conventional mass spectrometers. Intense lasers can ionize nearly all of the desorbed material, thereby dramatically increasing the detection efficiency. These laser ionization and particle ejection methods have been combined with recent advances in mass spectrometer design and optical imaging to produce several surface analysis instruments that feature capabilities found nowhere else in the world.

These instruments are being applied to a multitude of fundamental and applied surface analysis problems. Presently under investigation are (1) the origins of the universe as revealed through isotopic anomalies in meteorites, (2) the fundamentals of particle-solid interactions as studied via the yield and energy distribution of sputtered clusters, (3) ways of making better plastics by understanding diffusion of additives in polymers, (4) methods for directly measuring the solar wind composition by trace element analysis of collectors returned from space, (5) new techniques for making flat panel displays using self-assembled monolayers on surfaces, and (6) techniques for chemical imaging of various organic and inorganic materials, such as fracture surfaces.

787 MOLECULAR SIEVE MATERIALS--HETEROGENEOUS CATALYSTS

Chem.
Engr.
Mat. Sci.
Phy.
Theory

Molecular sieve materials in the aluminosilicate zeolite family and in the newer metalloaluminophosphate families are synthesized. Mechanistic aspects of their crystallization from gels are being investigated. Materials characterizations and studies of intrinsic properties are made with a variety of techniques, including X-ray diffraction and spectroscopy, neutron scattering, magnetic resonance spectroscopies, infrared spectroscopy, and electron microscopy. Molecular dynamics computer-simulation methods are being applied to the analysis of framework dynamics and to the siting and diffusive microdynamics of adsorbates in the intracrystalline pores. These properties control molecular shape-selectivity in both adsorption and catalysis. Ab-initio molecular-orbital theory is being used to investigate the Bronsted acid catalytic activity of the zeolites and their isomorphously-substituted analogues and conformations of molecules used as templates during gel crystallization. Materials made by intracrystalline encapsulation of transition-metal chalcogenide clusters or metallic clusters are being tested as novel catalyst formulations.

788 DIAMOND FILMS FROM FULLERENES

Diamond is an important material because of its exceptional hardness, high thermal conductivity, low electrical resistivity, chemical inertness, etc. Thus, there are many important applications where diamond films could be utilized, and a substantial amount of research is being conducted to learn how to produce high-quality thin diamond films. Such films are commonly grown using a hydrocarbon precursor in hydrogen gas. Hydrogen is generally believed to be necessary for the diamond thin-film growth process. However, hydrogen in varying amounts is inevitably incorporated in the growing diamond lattice, leading to structural defects. The growth of diamond films using fullerene (C_{60}) precursors in an argon microwave plasma without the addition of hydrogen or oxygen has recently been accomplished at Argonne National Laboratory. The gas mixtures were produced by flowing argon gas over fullerene-containing soot at high temperatures. Optical spectroscopy reveals that C_2 is present in the discharge, giving direct evidence that it is one of the products of C_{60} collisionally induced fragmentation. The nanocrystalline diamond films are characterized with scanning and high-resolution transmission electron microscopy, x-ray diffraction, and Raman spectroscopy.

789 THIN FILM GROWTH AND CHARACTERIZATION

Chem.
Comp. Sci.
Envr. Sci.
Phy.
Theory

The fabrication of thin film layered structures of multicomponent materials such as high-temperature and alloy superconductors, and ferro-electric and electro-optic materials, and the development of hybrid technologies incorporating some or all of these materials into a single device requires a detailed understanding of film growth and interface properties. In addition, the fabrication of reliable devices utilizing currently developing thin films technologies will require control of film properties at extremely sharp interfaces (one or two atomic layers). We have developed an instrument for performing pulsed beam time-of-flight ion scattering and recoil spectroscopy (TOF-ISARS) that permits real-time, in situ characterization of the growth layer of multicomponent oxide thin films with submonolayer resolution. This instrument is being used, for example, to study the deposition of Pb, Zr, Ti, and Ru using a sequential layer-by-layer deposition method under ambient oxygen pressure conditions appropriate for the growth of $PbZr_{1-x}Ti_xO_3$ films. Our measurements have shown layer-by-layer as well as two-dimensional and three-dimensional island growth during deposition. This and other systems of technological importance are currently under investigation.

790 AQUEOUS CORROSION

Chem.
Math.
Metal.
Phy.
Theory

The goal of this research is to elucidate fundamental aspects of the interfacial phenomena that occur on the surface of metals and metal oxides immersed in aqueous media. The conditions of study (temperature, pressure, and solution chemistry) cover domains that are applicable to corrosion in light-water nuclear reactors, ground-water interactions in nuclear waste storage environments, and the operation of fuel cells and batteries. The details that connect surface adsorption, electron transfer, and electrolyte chemistry with passive film structure are sought by a combination of in-situ surface-sensitive spectroscopic methods and transient electrochemical techniques. In-situ measurements using laser Raman and infrared spectroscopies are providing seminal information about electrochemical interfaces. Key features of the interfacial chemistry associated with passivation processes (including charge-transfer kinetics) are being studied by pulsed galvanostatic/potentiostatic, dc polarization, and ac-impedance techniques. A parallel theoretical effort seeks to simulate solid/liquid interface phenomena through the application of molecular dynamics methods in combination with ab initio molecular-orbital theory. The integration of high-temperature electrochemical kinetic measurements and surface spectroscopies with advanced theoretical methods is unique to our program, and continues to provide an improved fundamental understanding of pivotal interfacial processes in the field of energy production.

791 THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS

Chem.
Comp. Sci.
Math.
Phy.

In this project, experimental and theoretical studies are carried out to investigate important thermodynamic and structural properties of ordered solutions, amorphous (metastable) materials, strategic minerals, and chemical species that have significance for elevated-temperature corrosion processes. Fundamental thermodynamic measurements (e.g., emf) are combined with structural (e.g., neutron diffraction) and theoretical (e.g., molecular dynamics) studies to probe the solution behavior of ordered and associated liquids (e.g., chloroaluminates, "ionic" alloys, and silicates). Efforts are under way to extend this research to include Mössbauer and Extended X-ray Absorption Fine-Structure studies of the bonding properties of ordered phases at very low temperatures, i.e., below 25° K. Thermodynamic calculations based on statistical mechanical methods are applied to the computation of the thermodynamic characteristics of complex metallurgical media as well as corrosion processes. Electronic absorption spectroscopy and a variety of other physiochemical techniques, including X-ray diffraction, proton activation, and cyclic voltammetry are used to explore the dissolution of metals contained in domestic minerals and in industrial/energy by-products. Thermodynamical techniques are employed to determine enthalpies of formation, standard entropies, and Gibbs energies of formation of strategically-important minerals, fiber-optic materials, and fast-ion conducting glasses. Drop-calorimetric and vapor-pressure measurements are made on systems exhibiting metal-to-nonmetal transitions to develop a sound fundamental understanding of this important phenomenon.

MATHEMATICS AND COMPUTER SCIENCE DIVISION (MCS)

The Mathematics and Computer Science Division is a basic research division, where mathematicians and computer scientists collaborate to advance the state of the art of scientific computing. Our goals are to discover, adapt, and apply computational techniques that promise to be useful in solving scientific and engineering problems. In keeping with our goals, we choose selected applications to evaluate the methods, algorithms, and tools that we develop in our research activities. These applications may come from fluid mechanics, atmospheric science, materials science, molecular biology, or any other area of scientific interest where we believe that mathematics and computer science can advance the state of the art. Because parallel computers are playing an increasingly significant role in scientific computing, most of our research is directed toward parallel architectures.

ALGORITHMS AND SOFTWARE

An essential part of the MCS Division research program involves designing algorithms for the numerical solution of problems common to many scientific and engineering problems, and implementing these algorithms on high-performance computers.

792 NUMERICAL LINEAR ALGEBRA

Comp. Sci.
Linear Alg.
Math.

Efforts in numerical linear algebra focus on both theory and application. We are interested in the design and analysis of algorithms for solving large-scale problems on parallel architectures, with emphasis on the development of reusable software tools. Our current focus is on the solution of nonlinear algebraic equations arising in the solution of partial differential equations. These equations are used to model a variety of physical phenomena, including fluid flow and structural mechanics.
http://www.mcs.anl.gov/petsc/petsc.html

793 SENSITIVITY ANALYSIS AND DESIGN OPTIMIZATION

Appl. Math.
Appl. Engr.

Sensitivity analysis concerns itself with determining the change in responses of a computational model with respect to perturbations in certain key parameters. Furthermore, given a way to assess the sensitivity of model parameters to key parameters, one can then embed the model code in a numerical optimization procedure to find the values of input parameters that result in the desired model behavior. In this context, we are applying computational differentiation, optimization, and parallel programming techniques to problems as diverse as climate modeling, automotive manufacturing, aeronautics design, biomechanical engineering, disease modeling, and environmental assessment and remediation.
http://www.mcs.anl.gov/Projects/autodiff/

794 OPTIMIZATION

Comp. Sci. Optim. Compu. Math. Par. Comp.

Optimization research centers on the development of algorithms and software for the solution of large-scale optimization problems on high-performance computers. We are especially interested in optimization problems that arise in applications. Recent research activities have centered on the Toolkit for Advanced Optimization (TAO), a project to develop a new set of software components for the solution of large-scale problems. Other research activities involve interior-point methods, trust-region methods, global optimization, and software environments. Applications include computational crystallography and macromolecular modeling.

http://www.mcs.anl.gov/optimization

795 OPTIMIZATION TECHNOLOGY CENTER

Comp. Sci. Optim.

The Optimization Technology Center is operated jointly by Argonne and Northwestern University. Activities focus on the development of a network-enabled optimization library. Students will assist in the (1) development of network-resident tools to help users in problem formulation and software selection, and (2) the collection of case studies that show how optimization is used to solve real-world problems.

http://www.mcs.anl.gov/otc/

796 THE NETWORK-ENABLED OPTIMIZATION SYSTEM - NEOS

Comp. Sci. Optim. Par. Comp.

The NEOS Server is a novel environment for solving optimization problems over the Internet. There is no need to download an optimization solver, write code to call the optimization solver, or compute derivatives for nonlinear problems. The NEOS project uses modeling-language interfaces, software tools for remote usage and job processing, and automatic differentiation tools to compute derivatives. Students will develop and install new solvers for NEOS, and participate in the development of interfaces for the latest optimization solvers.

http://www.mcs.anl.gov/neos/Server

797 UNSTRUCTURED MESHES

Comp. Sci. Par. Comp. Unstruct. Mesh.

Our efforts are primarily in two research areas. The first is the development of new algorithms for the a priori improvement of unstructured meshes using local mesh smoothing techniques. We use optimization methods that are guaranteed to converge to an optimal solution at a low computational cost. We have shown that these techniques are robust, offer guaranteed improvement, and can be combined with other mesh improvement techniques to create high-quality simplicial meshes in both two and three dimensions. Research in this project includes the investigation of new optimization objective functions and the improvement and untangling of both simplicial and hexahedral meshes. This work has been encapsulated in the Opt-MS software, and more information can be found at: *http://www.mcs.anl.gov/~freitag/Opt-MS*

The second research area seeks to eliminate the barriers preventing application scientists from easily experimenting with independently developed mesh management software tools. A number of software tools exist that support parallel, adaptive mesh computations, but in each case a single style of mesh is supported and the application interface varies dramatically among the packages. By designing a component-based approach to mesh management tools, the application scientist writes to a single, standardized API and can then use any of the tools that are compliant with the standard. This work is part of the ALICE project at Argonne, and more information can be found at: *http://www.mcs.anl.gov/alice*

798 ALICE - ADVANCED LARGE-SCALE INTEGRATED COMPUTATIONAL ENVIRONMENT

Comp. Sci. Math. Par. Proc.

Many computational science simulations require a range of tools to address areas such as meshing, numerical partial differential equations, optimization, sensitivity analysis, and visualization. The integrated use of software libraries for these areas remains a challenge because of data management and interoperability issues. Within the Advanced Large-scale Integrated Computational Environment (ALICE) project, we are developing component-based infrastructure to enable integrated use of software developed independently by different groups, with particular emphasis on parallel and distributed computing. Potential projects include developing interfaces to libraries that support optimization, mesh generation, visualization, and collaboration. Additional projects support the interaction with other tools, such as computational differentiation and integrated computational workbenches.
http://www.mcs.anl.gov/Projects/alice/

COMPUTER SCIENCE

Computer science research addresses ways in which researchers can reduce the time required to write programs, increase their adaptability to high-performance computers, transform existing programs to derive sensitivity information, and enhance their clarity and correctness. For example, we are developing parallel-programming tools for transporting programs to new computer architectures. In addition, we continue to work with applications-oriented groups on projects such as computational biology.

799 COMPUTATIONAL DIFFERENTIATION

Comp. Sci.
Prog. Tools
Appl. Math.

Computational differentiation addresses the need of many disciplines of scientific computing for the accurate and efficient evaluation of gradients, Jacobians, or higher-derivative information. We are developing the ADIFOR, ADIC, and ADIC++ tools that, given an arbitrary program written in Fortran, C, or C++, automatically produce new code that accurately and efficiently computes designated derivatives of output parameters with respect to input parameters. We are also developing methodologies for exploiting mathematical structure of codes to be differentiated, in order to fully leverage the capabilities of these tools. This research is interdisciplinary and draws on compiler construction, graphical user interfaces, parallel computing, discrete algorithms, and analysis.

http://www.mcs.anl.gov/Projects/autodiff/

800 PARALLEL-PROGRAMMING TOOLS

Comp. Sci.
Graph. Tools
Par. Proc.

As parallel computers become more widely deployed and incorporate more complex architectures, the need for a software technology that allows a straightforward use of the next generation of parallel machines also increases. The focus of our research is the design of portable parallel libraries (MPI, Globus), the integration of multithreading and communication, the design and implementation of high-level languages (CC++), and interfaces to standard object brokers (CORBA). We also investigate applications in areas as diverse as environmental science, collaborative environments, computational chemistry, and medicine.

http://www.mcs.anl.gov/mpi
http://www.globus.org/

801 COMPUTATIONAL BIOLOGY

Comp. Bio.
Comp. Sci.
Logic Prog.

The objective of this research is to develop, implement, and use logic-based tools for the solution of scientific problems in molecular biology and genetics on high-performance computers. Current emphasis is on genetic sequence analysis and reconstruction of the metabolic network for sequenced genomes; tool development for automated analysis of metabolic models, and design of user-friendly querying tools to support research in biology and medicine.

http://wit.mcs.anl.gov/WIT2

802 AUTOMATED REASONING

Auto. Reas.
Comp. Sci.
Math.

Investigations are under way to develop new concepts and new applications for automated reasoning. Our emphasis is on the formulation of more effective ways of reasoning (inference rules) and more powerful strategies to control that reasoning. We also study various applications, including open questions from mathematics and logic.
http://www.mcs.anl.gov/AR/

803 MATHEMATICS OF PHYSICAL SYSTEMS

Anal. Meth.
Numer. Meth.
Math.

We are interested in nonlinear differential equations arising from the modeling of physical systems. Those currently studied come from condensed-matter physics and fluid dynamics and include the Ginzburg-Landau and Navier-Stokes equations. We explore the solutions of these equations through large-scale numerical simulations, apply scientific visualization techniques and postprocessing software to obtain qualitative and quantitative information, and use analytical methods where possible to interpret the results.
http://www-fp.mcs.anl.gov/division/research/applied_math.htm

804 PARALLEL I/O

Comp. Sci.
Compi-Lers
Par. Proc.

We are investigating scalable input/output techniques for high-performance computer systems. Research topics include the development of software support for high-performance I/O from scientific and other projects. Four projects are under way: (1) developing ROMIO, a portable implementation of MPI-IO (a standard API for parallel input/output); (2) developing scalable parallel I/O software for large (approximately 1000-node) Linux clusters; (3) combining techniques in parallel I/O and databases for large-scale scientific data management; and other applications; and (4) investigating the I/O capabilities of Java and using parallel I/O techniques to improve performance of Web servers.
http://www.mcs.anl.gov/romio *and http://www.mcs.anl.gov/~thakur*

805 HIGH-PERFORMANCE DISTRIBUTED COMPUTING

Comp. Sci.
Graphic Tools
Par. Proc.

The development of high-speed networks makes it possible to construct computations that integrate geographically distributed computers, databases, display devices, and other resources. We are investigating the protocols and tools required to support computing in large-scale internetworked environments. Topics include programming abstractions, security, resource naming and discovery, high-level languages, high-speed protocols, and applications in areas such as manufacturing and medicine.
http://www.globus.org/

806 WIDE-AREA PARALLEL COMPUTING

Comp. Sci.
Par. Proc.
Message Pass.

The Message Passing Interface (MPI) Standard is a widely used programmer's interface for writing parallel programs. It is particularly well suited to applications running on collections of computers that are in different buildings, cities, or countries. This project is enhancing the MPICH implementation of MPI (the most widely used implementation of MPI) to provide more efficient and robust communications in the wide-area environment. Projects include exploiting quality-of-service, support and better wide-area network protocols, and discovering the exploiting the topology of the network that the MPI application in running within.
http://www.mcs.anl.gov/mpi/mpich

807 MULTITHREADING IN NUMERICAL SOFTWARE

Comp. Sci.
Math.
Par. Proc.

Multithreading is a way to exploit multiple CPUs within a symmetric shared memory processor (SMP). It offers the potential for significant performance advantages over other parallelism strategies such as explicit message passing. This project will explore the use of multithreading in the PETSc numerical library. Because PETSc is aimed at solving large sparse linear and nonlinear systems that arise in the solution of partial differential equations, an effective multithreading implementation must take into account the structure and dynamic nature of the PETSc code. Techniques such as multicoloring and adaptive reorderings will be applied to develop an efficient implementation of key routines in PETSc.
http://www.mcs.anl.gov/petsc

COMPUTATIONAL SCIENCE

Computational science has joined theory and experiment as a third approach to solving scientific and engineering problems. We are addressing critical problems in areas such as climate modeling, environmental research, chemistry, materials science, and biology that require the use of high-performance computers and the development of new techniques to exploit those computers effectively.

808 CLIMATE MODELING

Clim. Model.
Comp. Sci.
Graph. Tools

Research focuses on the development of programming methodologies, algorithms, and graphics tools to support climate modeling on large parallel machines. This research is performed jointly with climatologists at the University of Wisconsin and at the National Center for Atmospheric Research, with the aim of understanding the effect of global change on climate at regional scales and on decadal time scales.
http://www.mcs.anl.gov/chammp/coupled/coupled_home.html

809 DYNAMICS OF VORTEX SYSTEMS

Comp. Sci.
Appl. Math.

We are applying high-performance parallel computing techniques to the study of high-temperature superconductors. Our goal is to better understand the mechanisms that determine the current-carrying capabilities of these materials and to simulate experimental techniques by which these capabilities can be improved. Because magnetic-flux vortices play a determining role, we focus on the dynamic properties of vortex systems in the presence of material inhomogeneities and defects.
http://www.mcs.anl.gov/Projects/super/sc_intro.html

810 SCIENTIFIC SONIFICATION

Comp. Sci.

In this research project we explore the use of sound for the analysis and exploration of complex data sets. We are developing DIASS++, a C++ version of DIASS (Digital Instrument for Additive Sound Synthesis). DIASS is a software system for the specification of a score and the generation of sound files from a score. DIASS++ will be used for the sonification of scientific data--the faithful rendition of scientific data through aural images (sounds). The data currently under investigation come from computational chemistry, computational superconductivity, and performance analysis of parallel computers.

http://www.mcs.anl.gov/Projects/music/index.html

811 COMPUTATIONAL CHEMISTRY

Comp. Sci.

Theor. Chem.

We are using quantum mechanical models to elucidate the geometric and electronic structures of large-scale molecular systems. Our applications include in-situ remediation of nuclear wastes and reaction probabilities for chemical reactions. These massive simulations are made possible by use of new (1) theoretical models that include relativistic effects, (2) scalable parallel algorithms, (3) software tools for efficiently utilizing modern teraflop-class computers, and (4) numerical analysis techniques (eigenanalysis and optimization) focused on these chemical applications.

http://www.mcs.anl.gov/grand-challenges/chem/index.html

812 CONSTRUCTION OF INTEGRATED BIOLOGICAL DATABASES

Integrat. Database

Genom. Info.

Logic. Prog.

We are constructing an integrated system, called WIT, that offers substantially enhanced access to the growing body of genomic information (e.g., chromosomes, sequence fragments, enzymes, and rRNA). The WIT project also involves development of new software tools, to support extraction of information from the integrated database. Our goal is to facilitate interpretation of genomes and to provide a valuable tool for scientists internationally.

http://wit.mcs.anl.gov/WIT2

813 NUMERICAL ALGORITHMS FOR FLOW SIMULATION

Comp. Sci.

Fluid Dynam.

We are exploring the development of parallel and high-order methods for computational fluid dynamics. This work includes the development of multilevel iterative solvers capable of scaling to thousands of processors, cache-aware computational kernels, and robust high-order numerical discretizations based upon spectral, spectral element, and WENO schemes. Applications include the study of transitional boundary layers, convection in deep atmospheres, and heat transfer enhancement mechanisms.

http://www-unix.mcs.anl.gov/appliedmath/Flow/cfd.html

COMPUTING FACILITIES

The MCS Division operates Argonne's Center for Computational Science and Technology, which features a scalable parallel IBM SP and SIG Origin 2000. A virtual reality environment has also been established, and activities are under way to integrate multimedia with high-performance computer systems.

814 SYSTEMS ADMINISTRATION

Comp. Sci. Network. Program. Comp. Envr.

The MCS Division computing environment consists of hundreds of UNIX computers, PCs running NT and Linux, and several supercomputers. Making these all work smoothly is a complex task, carried out by the MCS Systems Group. Students and visitors in the Systems Group take on special projects that enhance the computing environment, and also assist with day-to-day operations. Participants in the Systems Group can expect to learn a lot about how UNIX works, how NT works, and how to design and maintain large networks of computers.

http://www.mcs.anl.gov/computing/and http://www.mcs.anl.gov/systems/

Systems Administration

815 NETWORK ADMINISTRATION

Comp. Sci. Network. Program. Comp. Envr.

The computing environment in the MCS Division, which consists of hundreds of computers, is built on top of a modern-day high-performance network. The network includes ATM, HIPPI, and various types of ethernet and is implemented by using several different kinds of network equipment. The MCS Systems Group is responsible for building and monitoring the network and for helping it support both production computing and experimental research. Participants in the Systems Group who focus on networking can expect to build tools to help monitor the network, help to expand the network, manage and design network services, and diagnose problems.

http://www.mcs.anl.gov/computing/and http://www.mcs.anl.gov/systems/

Systems Administration

816 SYSTEMS PROGRAMMING

Comp. Sci. Network. Program. Comp. Envr.

The MCS Systems Group is responsible for managing the MCS computing environment, which consists of hundreds of computers. An important part of this environment is the design and development of new tools to support large-scale management. Members of the Systems Group who work as system programmers use Perl, Java, C, and various scripting languages to build new systems administration tools that are deployed within MCS and eventually released to the world at large. Participants can expect to learn appropriate programming languages, participate in the design of tools to help manage large scalability problems, and learn a great deal about how large environments of computers work.

http://www.mcs.anl.gov/computing/and http://www.mcs.anl.gov/systems/

Systems Admn.

817 VIRTUAL REALITY ENVIRONMENTS

Virtual Reality Envr. Network.

Virtual reality (VR) has become an increasingly familiar part of the visualization and communication of information. Collaborative VR environments at multiple sites are now being linked over high-speed networks with each site interacting with and viewing the results being discovered. This project uses the CAVE immersive VR environment as a testbed for developing shared VR tools, metrics, techniques, and protocols.
http://www.mcs.anl.gov/FUTURES_LAB/index.html

818 SCIENTIFIC VISUALIZATION AND SIMULATIONS INTERACTION IN AN IMMERSIVE VR ENVIRONMENT

Virtual Reality Envr. Network.

Virtual environments provide a powerful human-computer interface that opens the door to new methods of interaction with high-performance computing applications in several areas of research. We are interested in the use of virtual environments as a user interface to real-time simulations used in rapid prototyping procedures. Our projects center on visualization and interaction of models of Grand Challenge problems in computational chemistry, biology, materials science, and other disciplines.
http://www.mcs.anl.gov/FUTURES_LAB/index.html

819 MULTIMEDIA AND COLLABORATIVE ENVIRONMENTS

Comp. Sci.
Graph. Tools.
Comp. Network.

We are investigating the use of high-performance networking and computing resources to support collaborative research activities. Many fronts of research are active, including work in on-demand media servers, tools for local and wide-area scientific collaboration including linkages to advanced computation and visualization environments, and technology for advanced information resource management, involving toolkits for the development of intelligent agents, compression, indexing, and transaction monitoring for the World Wide Web.
http://www.mcs.anl.gov/FUTURES_LAB/

INFRASTRUCTURE FOR COLLABORATIVE ENVIRONMENTS

Virtual Envr.
Multi-media
Network.

The DOE2000 project integrates emerging multiuser virtual environment technology with state-of-the-art multimedia interfaces in order to support scientific collaboration. The resulting networked environment, composed of a persistent collection of objects and a flexible history mechanism, allows the creation of electronic virtual laboratories. These virtual laboratories will be networked locations where scientists interact with analytical electron microscopes, high energy physics experiments and data, and, most important, each other. This project is developing the tools to create these virtual laboratories and the scientists' interfaces and will validate these integrated tools in end-user testbeds.
http://www.mcs.anl.gov/DOE2000/

MULTIMEDIA SUPPORT FOR COLLABORATIVE ENVIRONMENTS

Virtual Envr.
Mult-media
Network.

The Voyager project seeks to develop the next-generation hypermedia server architecture that will enable the construction and rapid deployment of tools for building virtual environments. Voyager will provide an extensible environment for making audio, video, and other stream-oriented recordings available to others on the network. Voyager is what each user in a virtual organization will use to publish his/her information for the rest of the organization's users. It is being designed to be deployed both at the desktop level and also as a scalable server for high-performance media serving applications. Our goal is to use Voyager to explore the architecture for the next generation of collaborative environment tools and provide much-needed media server capability for collaborative environment infrastructure.
http://www.mcs.anl.gov/FUTURES_LAB/index.html

OFFICE OF PUBLIC AFFAIRS (OPA)

820 JOURNALISM AND PUBLIC RELATIONS OPPORTUNITIES

Journ.
Publ. Rel.
Sci. Writing

The Office of Public Affairs has internship opportunities for students interested in science-related journalism and public relations. The student would do "hands-on" activities in many areas of the Office of Public Affairs, including: preparing news releases reporting on scientific and technical advances at Argonne; assisting in the publication of the Argonne News, employee publications, and Logos, a quarterly scientific review. This internship requires a strong background in journalism and an interest in science. Articles generated during the internship are printed in Argonne publications with author credit and used in news-release form to scientific and general media.

PHYSICS DIVISION (PHY)

The Physics Division conducts basic experimental and theoretical research in nuclear, atomic, and molecular physics. We are also involved in the continuing development of the Argonne Tandem-Linear Accelerator System (ATLAS), a novel superconducting heavy-ion accelerator, which is operated as a national facility for nuclear physics research.

821 SUPERCONDUCTING HEAVY-ION LINAC "ATLAS"

Phy. Engr. Construction of the world's first superconducting heavy-ion accelerator is complete. This project has involved the development of a new technology. Operation of the accelerator will involve continuing upgrading tasks that are concerned with surface phenomena in rf resonators, cryogenic design, computer control, and the refinement of mechanical subsystems. Research participants would be able to choose from a wide variety of accelerator physics topics involving: superconducting rf cavities, ECR ion sources, control systems, beam transport, and linear-accelerator beam dynamics.

822 NUCLEAR REACTIONS AND NUCLEAR STRUCTURE STUDIES INDUCED BY HEAVY IONS

Phy. The interaction between nuclei is studied. Collisions are observed between accelerated heavy ions from the superconducting linac and target nuclei over the full periodic table up to and including uranium. These studies involve: elastic and inelastic scattering, heavy-ion resonances, nucleon transfer between colliding nuclei, compound-nucleus formation and fusion, particle and fission decay, gamma decay of high-spin states, nuclear astrophysics, and the production of nuclei far from stability. Also electron-positron production and other phenomena associated with the ultra-strong transient electromagnetic fields of two heavy nuclei passing each other are being investigated. In addition, the full accelerator system is used as an ultrasensitive mass spectrometer for radioisotope detection at very-low concentrations, with applications in various areas of physics and related research fields. Research participants could be involved in one or more of the experimental aspects of these studies which include, in addition to the accelerator system, particle detection techniques with solid-state and gas detectors, magnetic spectrometers and ion-beam optics, gamma-ray semiconductor detectors, picosecond time-of-flight, thin-foil target techniques, high-vacuum technology, multiparameter pulse electronics, and computer data handling and analysis.

823 NUCLEAR PHYSICS AT INTERMEDIATE ENERGIES

Phy. The strong interaction in nuclear matter is explored in these studies. In particular, the role of constituents of the nucleon such as mesons and quarks in a fundamental description of nuclear forces is examined primarily with electromagnetic probes. A new experimental program with CW electron beams has begun at the TJNAF (Thomas Jefferson National Accelerator Facility). The Argonne group constructed one of the pair of spectrometers which form the primary experimental equipment in the first operating experimental area at TJNAF. Higher energy experiments are underway at the Fermi National Accelerator Laboratory and at the HERA accelerator at DESY, Hamburg, Germany, which more directly probe quark degrees of freedom in nuclei. Among the new experimental equipment being developed for these studies is a laser-drive polarized hydrogen or deuterium target as an internal polarized target for storage ring experiments.

824 EXPERIMENTS WITH THE FRAGMENT MASS ANALYZER AND WITH GAMMASPHERE

Phy. GAMMASPHERE a national gamma-ray facility is used for detailed gamma-ray studies. Most studies focus on the properties of nuclei under extreme conditions of temperature, angular momentum and/or deformation. The Fragment Mass Analyzer (FMA) separates nuclear reaction products from the beam and transports them to a detector station. The device is used for a wide variety of applications focussing mostly on the properties of nuclei at the very limits of stability (N=Z nuclei, proton emitters, neutron-deficient and neutron-rich nuclei, superheavy elements, etc.).

825 THEORETICAL PHYSICS

Phy. The main objective of Argonne's nuclear theory research program is to develop fundamental understandings of nuclear dynamics under various conditions accessible to the experimental facilities at Argonne and other laboratories around the world. The principle areas of investigation are nuclear dynamics originating from mesonic and quark degrees of freedom, heavy-ion reactions, nuclear many-body problems, and nuclear structure. We are also actively investigating fundamental problems concerning the understanding of nuclear dynamics in terms of Quantum Chromodynamics.

REACTOR ANALYSIS DIVISION (RA)

This Division develops analytical methods and experimental techniques needed to ensure safe operation of fission reactors. The effort encompasses the analysis of the fuel cycle, core neutronics, fuel management, nuclear cross section data, feedback characteristics, lattice physics, potential accidents, reactor control, coolant dynamics, core structural safety, fuel-element damage propagation, fuel dynamics, fuel-coolant interactions, heat transfer, engineered safety features, and artificial intelligence based tools for surveillance and diagnosis.

To improve understanding of the safety and operation of liquid-metal-cooled reactors (LMRs) and light water-cooled reactors (LWRs), the Division conducts research and development to identify technology needs; investigates reactor physics and related issues, investigates safety questions and related phenomena; develops safety data, design methods, and criteria; and recommends appropriate safety philosophies.

The Division is also actively extending the methods and techniques it has developed for fission reactor operations to support research and development in many other fields such as the U.S. space program (NASA), coal-fired electric boilers, the automobile industry, and particle accelerators.

826 LARGE-SCALE COMPUTER CODE DEVELOPMENT

Comp. Sci.
Mech. Engr.
Nucl. Engr.

Large-scale computer codes for the analysis of steady-state performance and applied operational and accidental transients in reactor power plants are developed. Activities include (1) development of understanding of basic physical phenomena, (2) formulation of mathematical models, (3) development of numerical solution techniques for coupled, non-linear partial differential equation systems, (4) computer code programming (FORTRAN) and verification, (5) code and modeling validation (experiment analysis), and (6) code performance, improvement, maintenance, and graphics.

Model development and validation requires proficiency in one or more of the following disciplines: heat transfer, single and two-phase fluid dynamics, reactor physics, fuel management, nuclear data and engineering mechanics. Computer code development activities include numerical analysis methods, programming, and code verification and maintenance.

827 COMPUTER STUDIES OF NUCLEAR REACTORS

Comp. Sci.
Math.
Nucl. Engr.

Analyses are performed to predict the behavior of nuclear reactor systems in steady state or in operational and accidental transients. Large-scale computer codes containing models of heat transfer, single and two-phase flow, reactor neutron kinetics, reactor status, fuel depletion, ENDF/B data, and structural-mechanical behavior are employed. The participant should have a basic understanding of one or more of the following areas: heat transfer, fluid flow, reactor physics, fuel management, ENDF/B data, and a working knowledge of FORTRAN. Experience with large-scale scientific computer codes and applications is desirable.

828 PROBABILISTIC RISK ASSESSMENT

Math.
Mech. Engr.
Nucl. Engr.
Stat.

Probabilistic Risk Assessment (PRA) activities include development of probabilistic methods for applications to safety analysis of nuclear facilities including consequence analysis; basic plant component failure data analysis; systems reliability modeling with common cause failure; sensitivity theory methods and applications in PRA; use of PRA techniques in support of plants modifications and maintenance, including analysis of human factors in procedures; and applications of PRA methods and models to new facility designs with stress of spent fuel treatment and disposal facilities are carried out.

829 ARTIFICIAL INTELLIGENCE (AI) BASED PLANT CONTROL SYSTEMS

Comp. Sci.
Math.
Mech. Engr.

Activities include development of inductive learning methods for automated and systematic knowledge acquisition for diagnostic expert systems. Development of methods that accelerated learning for feedforward and recurrent artificial neural networks. Implementation of Monte Carlo based approaches, e.g., simulated annealing and genetic algorithms, as general-purpose control algorithms. Methodology developed may be tested in conjunction with the ANL-W Divisions at the ANL-W facilities.

830 ARTIFICIAL INTELLIGENCE APPLICATION

Comp. Sci.
Math.
Nucl. Engr.
Stat.

Large volumes of digitized data from operating nuclear power plants are processed, analyzed, and interpreted using state-of-the-art interactive techniques on distributed workstations and PCs. Software packages for various numerical, statistical, and time-series analyses are developed, modified, and maintained using a variety of languages and software-engineering tools. On-line expert systems are being developed that use automated reasoning techniques for assistance with the tasks of surveillance, diagnosis, and interpretation of physical parameters in advanced nuclear, aerospace, and industrial systems.

831 REACTOR SIMULATION AND CONTROLS LABORATORY

Comp. Sci.
Elec. Engr.
Math.
Nucl. Engr.

A reactor simulation and controls laboratory (RSCL) is developing high-performance network computing for coarse-grain parallelization and speedup of computationally-intensive reactor-simulation software on a network of Unix workstations. Activities include software engineering (C and Fortran languages); algorithmic analysis for identification of simulation processes amenable to parallelization; code decomposition, load balancing, synchronization, and timing studies on the network computing system; and design and integration of dynamic color-graphic human-machine interfaces to the simulation system.

832 MOLECULAR DYNAMICS COMPUTER CODE DEVELOPMENT

Comp. Sci.

Phy. Chem.

Chem. Phy.

Molecular dynamics simulation computer codes are developed to model chemical and physical interactions in media of interest to the nuclear waste management programs. The present focus is on the structure of zeolite containing a variety of chemical species, including clusters of radioactive fission products or actinides, anions, and other components, e.g., water. The interaction among the contained species and with the zeolyte framework is crucial to the development of zeolite as waste matrix materials. Activities include (1) validation of models and force parameters by comparison with neutron diffraction data and observed spectra, (2) visualization of simulation results to determine atomic locations (3) development of methods to determine macroscopic thermodynamic, chemical, and physical properties of zeolites embedded with other species, (4) computer code and visualization tool development, and (5) development or adaptation of parallel computing algorithms to enable very large simulations.

833 NEUTRON PHYSICS DATABASE APPLICATIONS IN MONTE CARLO

Nucl. Phy.

Comp. Sci.

Nucl. Engr.

Nuclear interaction datasets for continuous-energy Monte Carlo calculations are developed and enhanced. These are based on the Evaluated Nuclear Data File (ENDF) data, and require conversion of neutron resonance cross section parameters to rigorous continuous-energy cross section data and probability tables. Secondary energy and angle distributions must also be converted to probability tables for use in Monte Carlo simulation. Work is underway to perform the file conversions and to validate the new data by a variety of means, including comparison with benchmark critical assemblies and visual comparison of plots against standards. Activities include application of nuclear data processing codes, visualization tool development, and benchmarking of Monte Carlo simulations against experiment.

834 NUCLEAR WASTE AND REPOSITORY MODELING

Chem. Engr.

Comp. Sci.

Geol.

Mech. Engr.

The radiological characteristics of spent nuclear fuel and other potential waste forms are evaluated; and the impact of various waste processing techniques is assessed. The performance of nuclear wastes in a deep geological repository is modeled. Repository modeling must account for release of radionuclides from the waste package, and subsequent geochemical transport in the surrounding environment. Probabilistic risk evaluation tools are used to account for model and data uncertainties. Model development and validation requires an ability to integrate performance considerations from a wide variety of scientific fields. Experience with large-scale scientific and PRA computer codes is desirable.

Nucl. Engr.

835 FUEL PROCESS MODELING

Chem. Engr.

Mech. Engr.

Various chemical, thermal, and mechanical processes are involved in treating spent nuclear fuel and special nuclear materials to produce suitable waste forms for storage. Simulation of these processes is required to enable proper planning of the sequence of operations and material usage. Activities include development of a simulator for the overall process, including detailed models for the various processing steps, such as electrochemical transport and distillation. Data from the processes will be used to guide development of the models, especially in the area of process losses and material accountability.

836 NUCLEAR CRITICALITY SAFETY

Comp. Sci.

Math.

Nucl. Engr.

Criticality safety and shielding analyses are performed for complex configurations and operations involving wide ranges of geometries, materials, and neutron spectra. These analysis efforts employ state-of-the-art nuclear data libraries and software and are complemented by ongoing R&D in methods development, software development, critical experimental evaluation, safety analysis report preparation, and nuclear data library validation.

837 THE QUANTIFICATION OF FIT-FOR-SERVICE OF COMPONENTS VIA NEURAL AND STATISTICAL ANALYSIS

Comp. Sci.

Mat. Sci.

Nucl. Engr.

Stat.

The current confluence is exploited of the need for speedy design, operating, and marketing decisions, such as the reliability of new or in-service components, and the advances in computing the classification techniques. New computational intensive statistical techniques, and applications specific programming are applied which allow rapid assessment of performance based on very limited testing or operating data. Such analysis methodologies and tools provide input for a decision theoretic assessment of the fit-for-service, or risk in life extension of large systems with long design lifetimes, such as power plants, and enhance the competitiveness of products by estimating more realistic rates of degradation.

838 SAFEGUARDS ANALYSIS OF FISSILE NUCLEAR MATERIAL

Dec. Theory

Nucl. Engr.

Stat.

The safeguards activities include the development and testing of methods for the assessment and quantification of the precision and accuracy of instruments, the quantity and the probability of the material unaccounted for is accessed in light of possible diversion or in-process holdup. Of particular interest are nuclear facilities based on the electrometallurgical processing of spent nuclear fuel.

REACTOR ENGINEERING DIVISION (RE)

The Reactor Engineering (RE) Division conducts research and development in the engineering and material sciences, with concentration in nuclear technology and related sciences. Major areas of emphasis include research in nuclear safety technology, reactor and nuclear facility design, performance and safety evaluation, decontamination and decommissioning of nuclear facilities, and environmental management support.

This Division is responsible for a wide spectrum of technology development programs that require the integration of engineering disciplines in nuclear reactor technology. The Division has actively participated in applying its core competencies to programs in other fields of nuclear and non-nuclear technology. The major program areas in which the Division is involved in are nuclear energy, industrial interactions, non-proliferation and arms control, and environmental management support.

The Division conducts research and development by applying its engineering capabilities in system planning, design, computer simulation, modeling, analysis, experimentation, and production of engineering prototypes and components.

839 NUCLEAR DIAGNOSTICS IN ARMS CONTROL AND OTHER APPLICATIONS

Comp. Sci. Elec. Engr. Nucl. Engr. Phy.

The technologies developed in research often have useful application in verifying arms control treaties and other non-military applications, such as detection of contraband smuggling. Examples of technologies currently under development for both nuclear and non-nuclear treaty verification (such as START, CWC, CFE, and CTB) are radiation-detection instruments, neutron and gamma detectors, accelerators, electronic systems, and scanning-electron microscopes. These may be applied to counting missile reentry vehicles, measuring rocket-motor diameters, detecting nuclear warheads, determining chemical composition, or uniquely tagging military items. The objects of interest might contain fissionable materials, high-explosives, chemical agents, or other substances. Opportunities exist for contributions at any level in analysis, computations, and experiments, depending on current national concerns and on the experience and interests of the program participants.

840 MATERIALS BEHAVIOR

Engr.
Mech.
Mat. Sci.
Metal.
Nucl. Engr.

Efficient and reliable operation of a complex engineering system depends critically on the behavior of the materials from which its components are made. In this activity, the dependability of materials for such systems is established by extracting their key fundamental properties, developing an understanding of those properties in relation to the engineering application, and deriving models and performing experiments that allow extrapolation and prediction of the material's behavior under a variety of service conditions. Models for material behavior are often configured for incorporation in computer codes that follow the heat transfer and loading history along with the material's response. Methods are also explored for tailoring materials to fit particular applications. Historically, much of this effort was directed at the behavior of nuclear reactor fuel and cladding materials subjected to the thermal transients associated with the reactor environment. More recently, efforts have been directed toward a number of other diverse issues, including (1) assessing material properties for safety evaluations of foreign reactor designs, (2) tailoring steel railroad surfaces to mitigate crack propagation, (3) developing ductile titanium aluminide for aerospace applications, (4) studying the behavior of nuclear waste forms, (5) assessing the safety of composite flywheels, and (6) understanding irradiation embrittlement in connection with advanced light-water reactor designs and the extension of the life of existing reactors.

841 HEAT TRANSFER AND FLUID DYNAMICS

Chem. Engr.
Comp. Sci.
Mech. Engr.
Phy.

Analytical, experimental, and fundamental studies are being performed on a wide variety of heat-transfer and fluid-dynamics phenomena relevant to nuclear-reactor safety assessment. Areas currently under active investigation include two-phase flow modeling for LWR, safety analysis, basic studies on two-phase flow patterns and interfacial area, liquid-liquid explosions including vapor explosions, liquid-metal combustion, and radiative heat transfer in two-phase mixtures. High-speed motion-picture cameras and a flash X-ray system are available for experimental work.

842 COMPLEX INTEGRAL HEAT-TRANSFER ANALYSIS

Chem. Engr.
Mech. Engr.
Nucl. Engr.
Phy.

Many complex phenomena addressed are thermally driven. Ongoing efforts are developing appropriate analysis tools and techniques to address problems involving many geometric configurations and multiple modes of heat transfer. Current applications include thermal hydraulic behavior of full-scale systems and the apparatus used in medium- to large-scale experiments. For general configurations, integral heat-transfer modeling is performed within the SINDA code. For complex hydraulic systems, the FIDAP computational fluid dynamics code is used.

843 COMPUTER STUDIES IN ENGINEERING MECHANICS PROGRAM

Civil Engr.
Comp. Sci.
Engr. Mech.
Mech. Engr.
Nucl. Engr.

The program is concerned with the development of state-of-the-art computational mechanics tools and visualization tools with application to the solution of complex engineering mechanics problems found in industry and reactor safety analysis. Currently, we are doing research on the development of finite element computer engines for use on advanced computing architectures including a single workstation, a workstation cluster, scalable systems, and massively parallel computers. In addition, research has focused on using virtual reality tools, such as Argonne's immersive virtual reality CAVE to display computational mechanics results. Work in concurrent engineering is also being done. Another active research area is the development of numerical methods for evaluating the structural integrity of modern lightweight materials, such as fiberglass composites for potential use in automobiles and civil structures. Work is being done in seismic analysis with a particular focus on seismic isolation and sloshing of liquid-filled tanks. An ongoing research area is the simulation of the response of steel, reinforced concrete, and prestressed concrete structures to static and dynamic overpressure. Within this program, a strong effort is being applied to the simulation of various types of welding processes. Additional research areas include the following: fluid-structure interaction, thermomechanical analysis and high temperature response of concrete structures.

844 LIGHT-WATER REACTOR SAFETY ANALYSIS

Aeros. Sci.
Chem. Engr.
Comp. Sci.
Mech. Engr.
Nucl. Engr.
Phy.

A number of studies are under way involving various aspects of nuclear-reactor technology. These include studies of foreign reactor systems, studies of U.S. plant features, and modeling of the physical processes of postulated reactor accidents. The modeling activities closely coincide with ongoing laboratory experimental programs studying accident phenomena. The thermal-hydraulic, chemical interaction, and aerosol behavior of the real or simulated-core-melt materials are modeled in computer routines. The participants work with staff who are developing the physical models, creating computer routines, and integrating the computer models into large-scale, integrated computer codes.

845 ADVANCED REACTOR CONCEPT DEVELOPMENT

Comp. Sci.
Indus. Engr.
Mat. Sci.
Mech. Engr.
Nucl. Engr.

Opportunities exist for students to participate in development, analysis, and experiment activities supporting innovative concepts for future nuclear power plants. The advanced concepts emphasize passive safety, nonproliferation, long core lifetime, simplicity, low cost, and high reliability. Students will work with experienced researchers to study existing concepts, address new approaches, develop and utilize analytical models, and perform trade-off and optimizing studies. Specific disciplines of interest include heat transfer, fluid mechanics, materials science, heat exchanger technology, steam/gas turbine technology, and cost/efficiency modeling. Students may also select to participate in experiment activities including development of apparatus, assist staff in conducting experiments, interpret results, and compare data with model predictions.

846 QUANTITATIVE IMAGE ANALYSIS

Comp. Sci.
Elec. Engr.
Mat. Sci.

Examination of nuclear fuels and containment materials makes use of quantitative metallography performed on a PC-based image analysis system. Participants will measure metallurgical features observed in optical micrographs and electron-beam images and create figures for publication of the test results. Video clips of analytical and test results will be digitally captured from existing 8mm and VHS format videotapes and edited for presentation on the division's world wide web home page and at various meetings.

Mech. Engr. *Metal.* *Nucl. Engr.* *Phy.*

847 NUCLEAR FACILITY SAFETY ANALYSIS

Chem. Engr.
Mech. Engr.
Nucl. Engr.

The Facility Safety Section performs a variety of safety analyses for ANL non-reactor nuclear facilities. This activity involves studying the facility use, developing a catalogue of possible malfunctions that could result in the release of hazardous materials to the environment, and analyzing the consequences of the event, such as radiological doses to the public or workers. Mathematical models are developed to study the time-dependent behavior of accident-related parameters. Both personal computers and a Sun (UNIX) system are used, as necessary. In general, facility-specific codes may be developed as needed. Often, specific physical processes must be modeled for unique situations.

848 COMPUTER TECHNIQUES FOR POWER PLANT MANAGEMENT

Comp. Sci.

Math.

Nucl. Engr.

Phy.

Programs are in progress to apply advanced computer approaches to the diagnosis and management of transients at commercial-scale nuclear power plants. Techniques using elements of automated reasoning, expert systems and neural networks are being applied to identify and locate off-normal conditions in power plants as part of a joint study with an electrical utility partner. The PRODIAG code identifies transient conditions based on thermal-hydraulic principles and displays the problem area to the plant operator. This code is now operational, but is being expanded to identify multiple failure sites, to better define specific locations of faults, and to analyze a larger number of types of off-normal situations.

A second code (PROMANA) is being developed that will use the diagnosis provided by PRODIAG to develop recommendations for the plant operator to allow the operator to reconfigure the plant system to avoid the faulted section yet maintain operational capability if possible. This code will use plant schematics with thermal hydraulic properties of the plant systems to identify all possible alternative piping configurations and prioritize them before presenting recommendations to the operator.

Participants in this program are expected to have a strong computer programming background and will work with the staff to develop more efficient search algorithms, data analysis routines and an interactive display sequence to present results to the plant operators.

849 COMPUTATIONAL FLUID DYNAMICS

Chem. Engr.

Comp. Sci.

Elec. Engr. *Math.* *Mech. Engr.* *Nucl. Engr.* *Phy.*

Analysis is being performed on the fluid dynamics of a variety of large-scale engineered systems. Current efforts focus on, but are not limited to, problems related to nuclear safety. One area of interest is the behavior of coolant and molten fuel during severe hypothetical light-water nuclear-reactor accidents. Other efforts involve mass transfer issues during the high-temperature electro-chemical conditioning of nuclear waste. Analytical tools include the FIDAP code for fluid dynamics and heat- and mass-transfer.

TECHNOLOGY DEVELOPMENT DIVISION (TD)

The mission of the Technology Development (TD) Division is to support the research, development, and demonstration activities conducted within the Office of the Associate Laboratory Director for Engineering Research in five main areas:

- *EBR-II Spent Fuel Treatment*
- *Arms Control and Nonproliferation*
- *D&D Technologies and Applications*
- *Thermal Waste Processing Technologies*
- *Fusion*

In addition, a sixth area of new development initiatives in a variety of technologies is maintained which may grow into major areas themselves.

The most important mission is the EBR-II Spent Fuel Treatment. TD is responsible for this program which has as its objective a convincing demonstration of spent fuel conditioning and waste form development and production. TD also will produce or coordinate the production of new process equipment.

A second major mission is in Arms Control and Nonproliferation including an important Reduced Enrichment for Research and Test Reactors (RERTR) program. A primary objective is the development of high density, low enrichment fuel research and test reactors that can be used to replace the current HEU fuels in these reactors worldwide, thereby eliminating a significant nuclear proliferation pathway. The other objectives are the development of sensors, software and systems for nonproliferation and arms control applications and assist in policy analysis.

The Dismantlement, Deactivation, Decontamination, Decommissioning and Disposal (generally abbreviated as D&D) of aging nuclear facilities is a major strategic thrust area since it addresses a large problem for the DOE, US nuclear utilities and international organizations. The development of new technologies and their demonstrations on surplus ANL nuclear facilities and elsewhere form a key part of the work. The pilot D&D operations of the surplus nuclear facilities at ANL(E) are a second major part of the work performed by TD.

The Waste Management Technology mission addresses a major DOE thrust area. The Division's primary interest lies in the development and prototype usage of thermal waste processing devices. The objective is development and demonstration of technologies and technology transfer to the commercial sector.

In the fusion area, the Division manages the Interdivisional Fusion Power Program which is a significant member of the national fusion power development team. Our primary focus is in blanket technology, where we have the national lead role. The principal areas of work are liquid metal technology, advanced materials and first wall/blanket/shield design. The Fusion Power Program is also a member of the International Thermonuclear Experimental Reactor (ITER) team. A potential new initiative is the development, construction and operation of the Fusion Neutron Source.

In addition to these principal mission areas, there are a number of other areas in which technology development is being undertaken. These include use of advanced detection/interpretation techniques in a variety of applications (FAA, Drug Enforcement, Manufacturing), use of accelerators for neutron radiography, simulation in evolving advanced computing systems, and support to industrial initiatives.

850 APPLIED ACCELERATOR TECHNOLOGY

Comp. Sci.
Elect. Engr.
Phy.

These activities entail the development of advanced accelerator technology and require physics, engineering or computer programming support in the following areas:

(1) design and development of intense low-charge-state ion sources,
(2) design and development of accelerator-based neutron sources for neutron radiography or boron neutron capture therapy, and
(3) programming of mathematically-complex codes that model the dynamics of charged-particle beams.

851 INSTRUMENTATION APPLICATIONS

Nucl. Engr.
Phy.
Comp. Sci.

The use of neutrons and photons (gamma rays and x-rays) is being investigated for the nondestructive examination of luggage and cargo containers to detect illicit substances such as explosives, narcotics, currency, weapons, etc. These projects involve: modeling studies of neutron and photon interaction and transport, visualization of the data, development of algorithms for decision making, evaluation of nuclear data, and system studies. We are also investigating the use of neutrons and photons to characterize radioactive waste. There is also a program to develop radiation detectors and dosimetry methods in support of nuclear facility decontamination and decommissioning activities.

852 LASER APPLICATIONS LABORATORY

Phy.
Mat. Sci.
Mech. Engr.
Chem. Engr.

The laboratory focuses on collaborative research and development activities with industrial partners. The facility includes high-power industrial CO_2 and Nd:YAG lasers, five-axis workstations, and diagnostic systems for laser beam characterization, plasma analysis and process monitoring/control. A range of detectors are available for diagnostics and aerosol or spray characterization. Current collaborative research with industry include heat treating and glazing of steels, welding of metals and alloys, beam shaping and fiber optics and process monitoring. Other R&D activities include laser cladding, laser cutting and ablation in decommissioning and decontamination and materials testing using laser thermal simulation.

853 REDUCED ENRICHMENT FOR RESEARCH AND TEST REACTORS (RERTR)

Nucl. Engr.
Chem. Engr.

The DOE Office of Nonproliferation and National Security supports the activities of the Reduced Enrichment Research and Test Reactor (RERTR) program. The goal of the RERTR program is to minimize and eventually eliminate use of highly enriched uranium (HEU) in research and test reactors. The program has been very successful, and has developed low-enriched uranium (LEU) fuel materials and designs which can be used effectively in approximately 90 percent of the research and test reactors which used HEU of Western origin when the program began. Current activities focus on development of more advanced LEU fuels, collaboration with the Russian RERTR effort and other international participants in fuel development, development of an LEU-based process to produce MO-99, and technical assistance to research reactors wishing to convert to LEU.

854 AEROSOL SCIENCES

Chem. Engr.
Elec. Engr.
Envr. Engr.
Mech. Engr.
Phy.

Participants' primary responsibility will be to contribute to experimental investigations and theoretical modeling in the fields of basic and applied aerosol science. Opportunities also exist in the areas of computerized data acquisition and data reduction. Research applications include aerosol generation, transport, pollution control, sampling, and analysis for both nuclear and fossil power systems. Additional research areas involve the development of novel devices to disperse or collect particles or to develop instrumentation to measure aerosol parameters, pulsed corona applications, and spray generation and characterization. Basic areas of research include electrostatic particle charging, particle formation, transport, agglomeration, deposition, and adhesion mechanisms; radiative heat transfer in particle-laden gages; particle filtration; material erosion by aerosol impaction; aerosol-vapor interactions; and bioaerosol sampling and processing.

855 ADVANCED COMPUTING

Comp. Sci.
Mech. Engr.
Nucl. Engr.
Phy.

This research involves applying new advances in computing, such as parallel processing, distributed computing, distributed information systems, graphics in a distributed processing environment, and alternate programming models (e.g., object-oriented programming), to the development and application of improved system analysis, simulation, and information system capabilities. Additional work is being performed in automating the production of programs from high-level specifications in first-order logic. Current applications areas include development of an intelligent transportation simulator, a software reuse repository, and tools to support manufacturing process simulation Activities for participants include algorithm and model development, programming GUI's, DBMs development, and data communications. Familiarity with C, FORTRAN, UNIX and X11/Motif, logic, and functional programming are desirable.

856 ARMS CONTROL AND NONPROLIFERATION TECHNOLOGY AND POLICY

Elec. Engr.
Mech. Engr.
Nucl. Engr.
Phy.

Argonne's multidisciplinary work in the field of arms control and nonproliferation technology and policy is coordinated through the Arms Control and Nonproliferation Program, which is run from the Technology Development Division.

Within this program, people with many skills, including chemists, physicists, engineers, material scientists, and even attorneys, work together to support U.S. government efforts to control weapons of mass destruction and to prevent their spread. Program staff support arms control treaty negotiation, implementation, and verification. They develop technology for on-site inspection and remote sensing, material/item identification, tracking shipments, and detection and prevention of nuclear proliferation. Staff members are also actively pursuing a study of alternative uses and destruction options for weapons materials.

857 BLANKET AND SHIELD STUDIES

Chem.
Chem. Engr.
Mat. Sci.
Mech. Engr.

This activity is concerned with a general design evaluation of first wall/blanket/shield components of fusion reactors. Various combinations of blanket structural material/coolant/tritium breeding material are being reviewed to develop a well-defined set of design criteria. Experimental and analytical activities on first-wall, blanket, and shield components are underway to develop design tools for reactor first-wall, blanket, and shield including neutronics, thermal hydraulics, and structural mechanics. A key area is the investigation of liquid metal magnetohydrodynamic effects of flowing liquid metals in a magnetic field.

Metal. Engr. *Nucl. Engr.*

858 FUSION MATERIALS STUDIES

Comp. Sci.
Elec. Eng.
Math.

Investigations are conducted to develop an understanding of the effects of a fusion-reactor environment on the properties and performance of candidate structural materials. These efforts are focused on low-activation vanadium alloys and include investigations of irradiation effects, corrosion/compatibility, mechanical properties and welding. This activity includes evaluation and correlations of fission-reactor and ion irradiations to simulate the displacement damage and transmutation reactions characteristic of a fusion neutron spectrum.

Nucl. Engr. *Phy.*

859 FUSION BLANKET MATERIALS AND TECHNOLOGY TESTING

Nucl. Engr.
Phy.
Mat. Sci.

This research involves development and testing of materials and fundamental technologies required for tritium breeding blankets. An important aspect of this effort is the development of electrically insulating coatings on a vanadium alloy structure to mitigate magnetohydrodynamic effects associated with a flowing liquid metal in high magnetic fields. This activating includes development of ceramic breeding materials, tritium recovery from liquid and ceramic breeding materials and neutronic analysis of tritium breeding capability, activation and afterheat of irradiated materials, and shielding characteristics.

860 PLASMA/MATERIAL INTERACTION RESEARCH

Mech. Engr.
Metal. Engr.
Nucl. Engr.

A variety of studies are underway to develop physics models and computer codes to study reactor conditions in magnetic-fusion devices. Current emphasis is on plasma materials interactions in tokamak devices, plasma heating and current drive, and overall power balance and operating conditions. Specific studies include sputtering erosion/redeposition, disruption modeling and analysis, and hydrogen isotope diffusion and inventory in first wall and divertor materials.

861 LIQUID METAL TECHNOLOGY FOR FUSION

Comp. Sci.
Elec. Engr.

This project involves several related areas of liquid metal technology for fusion. An electrically insulating coating is needed to reduce the magnetohydrodynamic (MHD) pressure drop in a liquid lithium blanket cooling system. Theoretical modeling of liquid metal flows inside magnetic fields within coolant ducts having electrically non-conducting and conducting walls is being developed. Equipment necessary for applying and testing electrically insulating coatings is being designed and developed. The main thrust of all activities in this area are directed towards developing and applying an insulator coating to a new vanadium alloy test section for MHD pressure drop testing in ANL's ALEX (Argonne Liquid-Metal Experiment) facility.

862 FUSION ENGINEERING RESEARCH

Chem. Engr.
Elec. Engr.
Mech. Engr.
Nucl. Engr.

The project involves design and analysis of fusion power systems. The International Thermonuclear Experimental Reactor (ITER) is a near-term device scheduled to begin construction in 2000. Argonne is involved in the design of in-vessel components including the shield/blanket, start-up limiters, and divertor. Activities include design analyses in the areas of thermalhydraulics, thermo-mechanics, neutronics, dynamic mechanical response, materials behavior, and performance/lifetime limits. This activity includes the design of advanced fusion power systems that operate at high power densities and high temperatures with extended lifetimes involving use of liquid metals as coolant/breeding material, advanced structural materials such as vanadium alloys and SiC composites, and novel energy conversion systems that can achieve high conversion efficiency.

863 SPENT NUCLEAR FUEL PROCESSING

Comp. Sci.
Chem. Engr.
Chem.
Nucl. Engr.
Metal. Engr.

Pilot Scale - Demonstration of electrometallurgical technology for metallic fast reactor fuel from EBR-II is being conducted at the Fuel Conditioning Facility. This technology employs a combination electrochemical and metallurgical process to prepare spent nuclear fuel for disposal. Processing takes place in a heavily shielded argon-atmosphere cell. Process control is automated to the extent possible through the use of computer and programmable logic controllers. Areas of research include computer modeling of the pyroprocesses and engineering of improved equipment with faster process rates and greater automation.